

Convergence of infinite element methods for scalar waveguide problems

Thorsten Hohage

Lothar Nannen

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Abstract

We consider the numerical solution of scalar wave equations in domains which are the union of a bounded domain and a finite number of infinite cylindrical waveguides. The aim of this paper is to provide a new convergence analysis of both the Perfectly Matched Layer (PML) method and the Hardy space infinite element method in a unified framework. We treat both diffraction and resonance problems. The theoretical error bounds are compared with errors in numerical experiments.

1 Introduction

We consider the numerical solution of time harmonic wave equations in domains which are the union of some bounded interior domain and a finite number of semi-infinite waveguides (see Fig. 1). We consider both the case of excitation by incoming propagating modes in one of the waveguides or by a source in the interior domain and the case of resonance problems. For the analysis of existence, uniqueness and properties of solutions to such problems we refer to [1, 23] and the references therein.

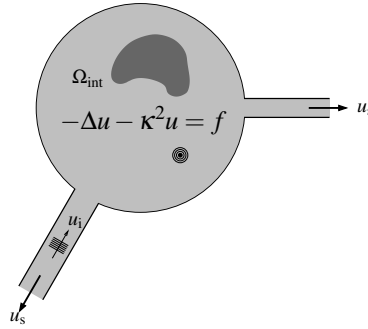


Figure 1: sketch of the waveguide problem under consideration

If such problems are solved numerically by finite element methods, the waveguides require a special treatment to avoid reflections at artificial boundaries in the waveguides. A simple option is to precompute the propagating modes by solving an eigenvalue problem on the cross section of each waveguide and use this to construct an approximation to the Dirichlet-to-Neumann map. However, the Dirichlet-to-Neumann map depends in a non-polynomial way on the wave number. For resonance problems this destroys the eigenvalue structure of the problem. Nevertheless, there exist alternative numerical methods for waveguide resonance problems, e.g. using Greens functions [25] or eigenfunction expansions in the interior domain [19, 24].

In this paper we analyze the convergence of numerical methods which are based on a variational formulation in the waveguides. We present two general convergence theorems based on S-coercivity arguments [3]. It is used to prove both convergence of the Perfectly Matched Layer (PML) method and the Hardy space infinite element method (HSM). This is the first complete convergence analysis of the Hardy space method in dimension greater than 1. Moreover, it differs from previous convergence results for the PML method [1, 5, 13, 14, 16, 18] in the fact that the truncation of the PML layer (with Dirichlet boundary conditions) is treated as an approximation error, not as an error on a continuous level. In this sense we interpret PML as an infinite element method, i.e. as a conforming discretization of a variational formulation of the original problem on an unbounded domain. Therefore no modeling error has to be taken into account. Moreover, it gives rise to a unified treatment of PML and HSM. Finally, we discuss a method to treat frequencies close to Wood anomalies by the Hardy space method.

The plan of this paper is as follows: After a general formulation of the problem in Sec. 2 we state in Sec. 3 the main convergence theorems for diffraction and resonance problems in an abstract framework, which are proved in Sec. 4. In the following we apply the convergence theorems to the PML (Sec. 5) and to the Hardy space method (Sec. 6) both for scalar Helmholtz diffraction and resonance problems. In the last section we give numerical convergence studies for the Hardy space method and show that the method is applicable to resonance problems.

2 Formulation of the problem

Let $\Omega = \Omega_{\text{int}} \cup \bigcup_{l=1}^L (W_l \cup \Gamma_l) \subset \mathbb{R}^d$ be a Lipschitz domain, which is the disjoint union of a bounded Lipschitz domain Ω_{int} , L semi-infinite cylinders (waveguides) W_1, \dots, W_L and interfaces Γ_l . More precisely, the W_l and Γ_l are of the form $W_l = \eta_l((0, \infty) \times \tilde{\Gamma}_l)$ and $\Gamma_l := \eta_l(\{0\} \times \tilde{\Gamma}_l)$ where $\eta_l : \mathbb{R}^d \rightarrow \mathbb{R}^d$ is a Euclidean motion and $\tilde{\Gamma}_l \subset \mathbb{R}^{d-1}$ is a bounded Lipschitz domain. The interfaces are assumed to be contained in $\overline{\Omega_{\text{int}}}$. The exterior domain is defined as $\Omega_{\text{ext}} := \bigcup_{l=1}^L W_l$.

For the sake of simplicity of exposition we will consider the standard Helmholtz equation in all our examples. However, we will formulate our convergence results in an abstract framework which includes certain variable coefficients in the interior domain

and in the lateral directions of the waveguides. Consider the diffraction problem

$$-\Delta u - \kappa^2 u = f \quad \text{in } \Omega \quad (2.1a)$$

$$\mathcal{B}u = g \quad \text{on } \partial\Omega \quad (2.1b)$$

$$u - u^{\text{inc}} \quad \text{satisfies a radiation condition in } \Omega_{\text{ext}}. \quad (2.1c)$$

Here $\kappa > 0$ is a given wave number, \mathcal{B} is a trace operator, e.g. the Dirichlet trace operator $\mathcal{B}u = u|_{\partial\Omega}$ or the Neumann trace operator $\mathcal{B}u = \frac{\partial u}{\partial \nu}|_{\partial\Omega}$, and we assume that $\text{supp } f$ and $\text{supp } g$ are contained in $\overline{\Omega_{\text{int}}}$. Moreover, u^{inc} is some given incident field in Ω_{ext} satisfying $(\Delta + \kappa^2)u^{\text{inc}} = 0$ in Ω_{ext} and $\mathcal{B}u^{\text{inc}} = 0$ on $\partial\Omega_{\text{ext}} \setminus \bigcup_{l=1}^L \Gamma_l$. The terms radiation condition and incident will be defined in Definition 2.1 below.

We will also consider resonance problems, which have the form (2.1), but f, g , and u^{inc} vanish, κ may be complex valued, and both κ and $u \neq 0$ are considered as unknowns.

In this paper we will consider several equivalent formulations of the radiation condition leading to different numerical algorithms. We start with the most standard one based on a series expansion of the solution. We may assume w.l.o.g. that $W_l = \{0\} \times \tilde{\Gamma}_l$ for some $l = 1, \dots, L$ (otherwise change to the coordinate system given by η_l). Moreover, we assume that the coefficients of \mathcal{B} are constant on W_l and that the negative Laplacian $-\Delta_l : \mathcal{D}(-\Delta_l) \subset L^2(\tilde{\Gamma}_l) \rightarrow L^2(\tilde{\Gamma}_l)$ with a domain of definition $\mathcal{D}(-\Delta_l)$ incorporating \mathcal{B} is self-adjoint and has a compact resolvent. For the Dirichlet trace operator this is the case with $\mathcal{D}(-\Delta_l) = H^2(\tilde{\Gamma}_l) \cap H_0^1(\tilde{\Gamma}_l)$, and for the Neumann trace operator with $\mathcal{D}(-\Delta_l) = \{v \in H^2(\tilde{\Gamma}_l) : \frac{\partial v}{\partial \nu} = 0 \text{ on } \partial\tilde{\Gamma}_l\}$. Then there exists a complete orthonormal set $\{\varphi_n : n \in \mathbb{N}\} \subset L^2(\tilde{\Gamma}_l)$ of eigenfunctions, $-\Delta_l \varphi_n = \lambda_n \varphi_n$ with $\lambda_n \geq 0$. (Here and in the following we omit the index l .) We generally assume in this paper that

$$\kappa^2 \notin \bigcup_{l=1}^L \sigma(-\Delta_l). \quad (2.2)$$

Then by separation of variables every solution to (2.1a) and (2.1b) with $\kappa > 0$ has the form

$$u(x, y) = \sum_{n=1}^{\infty} (c_n \exp(i\kappa_n x) + d_n \exp(-i\kappa_n x)) \varphi_n(y) \quad \text{in } W_l \quad (2.3)$$

where c_n and d_n are complex coefficients, $x \in (0, \infty)$, $y \in \tilde{\Gamma}_l$ and

$$\kappa_n := \begin{cases} \sqrt{\kappa^2 - \lambda_n}, & \kappa^2 > \lambda_n \\ i\sqrt{\lambda_n - \kappa^2}, & \kappa^2 < \lambda_n \end{cases}. \quad (2.4)$$

The functions $\exp(i\kappa_n x)\varphi_n(y)$ and $\exp(-i\kappa_n x)\varphi_n(y)$ are called waveguide modes. If $\kappa^2 < \lambda_n$, then $\exp(-i\kappa_n x)$ is exponentially growing as $x \rightarrow \infty$ whereas $\exp(i\kappa_n x)$ is exponentially decaying. The functions $\exp(i\kappa_n x)\varphi_n(y)$ are called *evanescent modes*. Since we expect a physical solution to be bounded, we require that $d_n = 0$ for such n . The modes $\exp(\pm i\kappa_n x)\varphi_n(y)$ with $\kappa^2 > \lambda_n$ are called *propagating modes*. Since $\lim_{n \rightarrow \infty} \lambda_n = \infty$ every waveguide W_l supports at most a finite number of propagating

modes. If the time dependence is given by $\exp(-i\omega t)$ then $\exp(i(\kappa_n x - \omega t))$ is propagating to the right whereas $\exp(-i(\kappa_n x + \omega t))$ is propagating to the left. Moreover, if u is an acoustic and transverse magnetic electric field, then $\mathcal{J}_l(u) = \Im \int_{\Gamma_l} \bar{u} \frac{\partial u}{\partial x} ds$ can be interpreted as average outward energy flux through Γ_l , and $\mathcal{J}_l(e^{i\kappa_n x} \phi_n(y)) > 0$ whereas $\mathcal{J}_l(e^{-i\kappa_n x} \phi_n(y)) < 0$. Therefore, we call $\exp(i\kappa_n x) \phi_n(y)$ an *outward propagating mode* and $\exp(-i\kappa_n x) \phi_n(y)$ an *inward propagating mode*.

Definition 2.1 (modal radiation condition). *Let u be a solution to (2.1a) and (2.1b) with $\kappa > 0$ and assume (2.2). We say that u satisfies the (modal) radiation condition if it is a linear combination of evanescent and outward propagating modes in each waveguide W_l , $l = 1, \dots, L$. u is called an incident field if it is a linear combination of inward propagating modes in each waveguide W_l , $l = 1, \dots, L$.*

3 Formulation of the main convergence theorems

We first formulate the assumptions of our general convergence theorem. To illustrate and motivate these assumptions we show in this section that they are satisfied in the simplest case

$$\kappa^2 < \inf \bigcup_{l=1}^L \sigma(-\Delta_l), \quad (3.1)$$

i.e. that none of the waveguides supports a propagating mode. We assume that \mathcal{B} is the Dirichlet trace operator $g = 0$, and of course $u^{\text{inc}} = 0$. Moreover, let $L = 1$ and $W := (0, \infty) \times \tilde{\Gamma}$ and set $W := W_1$, $\tilde{\Gamma} := \tilde{\Gamma}_1$, and $\Delta_{\tilde{\Gamma}} := \Delta_1$. Then we obtain the following variational formulation of (2.1) in $\mathcal{V} = H_0^1(\Omega)$:

$$\int_{\Omega} (\nabla u \cdot \nabla \bar{v} - \kappa^2 u \bar{v}) dx = \int_{\Omega_{\text{int}}} f \bar{v} dx \quad (3.2)$$

Assumption A: Exterior and interior spaces. *Let \mathcal{V}^{int} and \mathcal{V}^{ext} be two Hilbert spaces, let \mathcal{Z} be another Hilbert space (a trace space), and consider bounded, linear, surjective (trace) operators $\text{tr}_+ : \mathcal{V}^{\text{ext}} \rightarrow \mathcal{Z}$ and $\text{tr}_- : \mathcal{V}^{\text{int}} \rightarrow \mathcal{Z}$. We set*

$$\mathcal{V} := \left(\begin{pmatrix} u^{\text{int}} \\ u^{\text{ext}} \end{pmatrix} \in \mathcal{V}^{\text{int}} \oplus \mathcal{V}^{\text{ext}} : \text{tr}_+ u^{\text{ext}} = \text{tr}_- u^{\text{int}} \right).$$

Moreover, there exist Hilbert spaces $\mathcal{X}_l^1, \mathcal{X}_l^2, \mathcal{Y}_l^1$, and \mathcal{Y}_l^2 for $l = 1, \dots, L$ such that $\mathcal{X}_l^2 \subset \mathcal{X}_l^1$ and $\mathcal{Y}_l^2 \subset \mathcal{Y}_l^1$ are densely and continuously embedded, and

$$\begin{aligned} \mathcal{V}^{\text{ext}} &= \bigoplus_{l=1}^L \mathcal{V}_l^{\text{ext}}, & \mathcal{V}_l^{\text{ext}} &:= \mathcal{X}_l^2 \otimes \mathcal{Y}_l^1 \cap \mathcal{X}_l^1 \otimes \mathcal{Y}_l^2, \\ \langle u^{\text{ext}}, v^{\text{ext}} \rangle_{\mathcal{V}^{\text{ext}}} &= \sum_{l=1}^L \left(\langle u_l^{\text{ext}}, v_l^{\text{ext}} \rangle_{\mathcal{X}_l^2 \otimes \mathcal{Y}_l^1} + \langle u_l^{\text{ext}}, v_l^{\text{ext}} \rangle_{\mathcal{X}_l^1 \otimes \mathcal{Y}_l^2} \right). \end{aligned} \quad (3.3)$$

Finally, let $s^{\text{int}} : \mathcal{V}^{\text{int}} \times \mathcal{V}^{\text{int}} \rightarrow \mathbb{C}$ and $s^{\text{ext}} : \mathcal{V}^{\text{ext}} \times \mathcal{V}^{\text{ext}} \rightarrow \mathbb{C}$ be bounded sesquilinear forms and set

$$s : \mathcal{V} \times \mathcal{V} \rightarrow \mathbb{C}, \quad s \left(\begin{pmatrix} u^{\text{int}} \\ u^{\text{ext}} \end{pmatrix}, \begin{pmatrix} v^{\text{int}} \\ v^{\text{ext}} \end{pmatrix} \right) := s^{\text{int}}(u^{\text{int}}, v^{\text{int}}) + s^{\text{ext}}(u^{\text{ext}}, v^{\text{ext}}).$$

As a closed subspace of $\mathcal{V}^{\text{int}} \oplus \mathcal{V}^{\text{ext}}$ the space \mathcal{V} equipped with the scalar product $\left\langle \begin{pmatrix} u^{\text{int}} \\ u^{\text{ext}} \end{pmatrix}, \begin{pmatrix} v^{\text{int}} \\ v^{\text{ext}} \end{pmatrix} \right\rangle_{\mathcal{V}} := \langle u^{\text{int}}, v^{\text{int}} \rangle_{\mathcal{V}^{\text{int}}} + \langle u^{\text{ext}}, v^{\text{ext}} \rangle_{\mathcal{V}^{\text{ext}}}$ is a Hilbert space. The spaces \mathcal{X}_l^j correspond to the infinite directions of the waveguides whereas \mathcal{Y}_l^j correspond to the cross sections.

Remark 3.1. $\mathcal{V}_l^{\text{ext}}$ is a subset of the tensor product Hilbert space $\mathcal{X}_l^1 \otimes \mathcal{Y}_l^1$, which is defined via completion under the scalar product

$$\langle u_1 \otimes v_1, u_2 \otimes v_2 \rangle_{\mathcal{X}_l^1 \otimes \mathcal{Y}_l^1} := \langle u_1, u_2 \rangle_{\mathcal{X}_l^1} \langle v_1, v_2 \rangle_{\mathcal{Y}_l^1}, \quad u_1, u_2 \in \mathcal{X}_l^1, \quad v_1, v_2 \in \mathcal{Y}_l^1.$$

Hence, $u \otimes v \in \mathcal{V}_l^{\text{ext}}$ is well defined. But $\mathcal{V}_l^{\text{ext}}$ is not a tensor product Hilbert space due to the definition of the scalar product in (3.3).

Verification for (3.2): Assumption A is satisfied if we split $u \in H_0^1(\Omega)$ into $u^{\text{int}} := u|_{\Omega_{\text{int}}}$ and $u^{\text{ext}} := u|_{\Omega_{\text{ext}}}$. More precisely, we have for the exterior space

$$\begin{aligned} \mathcal{X}^1 &:= L^2((0, \infty)), & \mathcal{X}^2 &:= H^1((0, \infty)), & \mathcal{Y}^1 &:= L^2(\tilde{\Gamma}), & \mathcal{Y}^2 &:= H_0^1(\tilde{\Gamma}), \\ \mathcal{V}^{\text{ext}} &:= \mathcal{X}^2 \otimes \mathcal{Y}^1 \cap \mathcal{X}^1 \otimes \mathcal{Y}^2 \sim \{u^{\text{ext}} \in H^1(\Omega_{\text{ext}}) : u^{\text{ext}}|_{\partial\Omega_{\text{ext}} \setminus \Gamma} = 0\}, \end{aligned}$$

with norms $\|u\|_{\mathcal{X}^2}^2 := \|u\|_{L^2}^2 + \|u'\|_{L^2}^2$ and

$$\|u\|_{\mathcal{Y}^2}^2 := \|u\|_{L^2}^2 + \|\nabla u\|_{L^2}^2 = \langle u - \Delta_{\tilde{\Gamma}} u, u \rangle_{L^2} = \|(\mathbf{I} - \Delta_{\tilde{\Gamma}})^{1/2} u\|_{L^2}^2,$$

such that the norm defined by (3.3) is given by $\|u\|_{\mathcal{V}^{\text{ext}}}^2 = 2\|u\|_{L^2(\Omega_{\text{ext}})}^2 + \|\nabla u\|_{L^2(\Omega_{\text{ext}})}^2$. Moreover,

$$\begin{aligned} \mathcal{V}^{\text{int}} &= \{u^{\text{int}} \in H^1(\Omega_{\text{int}}) : u^{\text{int}}|_{\partial\Omega_{\text{int}} \setminus \Gamma} = 0\}, \\ \mathcal{Z} &= H_0^{1/2}(\Gamma) = \mathcal{D}\left((\mathbf{I} - \Delta_{\Gamma})^{1/4}\right), \quad \text{tr}_- u^{\text{int}} := u^{\text{int}}|_{\Gamma}, \quad \text{tr}_+ u^{\text{ext}} := u^{\text{ext}}|_{\Gamma}, \\ s^{\text{int}}(u^{\text{int}}, v^{\text{int}}) &= \int_{\Omega_{\text{int}}} \left(\nabla u^{\text{int}} \cdot \nabla \overline{v^{\text{int}}} - \kappa^2 u^{\text{int}} \overline{v^{\text{int}}} \right) dx, \\ s^{\text{ext}}(u^{\text{ext}}, v^{\text{ext}}) &= \int_{\Omega_{\text{ext}}} \left(\nabla u^{\text{ext}} \cdot \nabla \overline{v^{\text{ext}}} - \kappa^2 u^{\text{ext}} \overline{v^{\text{ext}}} \right) dx. \end{aligned}$$

In the following we will assume that \mathcal{Z} is equipped with the inner product $\langle u, v \rangle_{\mathcal{Z}} := \sum_{n=1}^{\infty} (1 + \lambda_n)^{1/2} \langle u, \varphi_n \rangle \langle \varphi_n, v \rangle$.

Assumption B: separation of \mathcal{V}^{ext} . There exists a complete orthogonal system $\{\varphi_n : n \in \mathbb{N}\} \subset \bigoplus_{l=1}^L \mathcal{Y}_l^2$ with the following properties:

1. For all $n \in \mathbb{N}$ we can choose $l(n) \in \{1, \dots, L\}$ such that for $\varphi_n = (\varphi_n^{(1)}, \dots, \varphi_n^{(L)})$ it holds $\varphi_n^{(j)} = 0$ for $j \neq l(n)$.
2. The subspaces (not to be confused with $\mathcal{V}_l^{\text{ext}}$ of Ass. A)

$$\mathcal{V}_n := \mathcal{X}_{l(n)}^1 \otimes \text{span}\{\varphi_n\} \cap \mathcal{V}^{\text{ext}}$$

are orthogonal in \mathcal{V}^{ext} both with respect to the inner product of \mathcal{V}^{ext} and with respect to s^{ext} , and the spaces $\text{tr}_+(\mathcal{V}_n)$ are orthogonal in \mathcal{Z} .

3. Finally, $\dim \text{tr}_+(\mathcal{V}_n) < \infty$ for all $n \in \mathbb{N}$ and

$$\mathcal{V}^{\text{ext}} = \bigcup_{n \in \mathbb{N}} \mathcal{V}_n \quad \text{and} \quad \mathcal{Z} = \bigcup_{n \in \mathbb{N}} \text{tr}_+(\mathcal{V}_n).$$

It follows from the assumption $\mathcal{V}^{\text{ext}} = \bigcup_{n \in \mathbb{N}} \mathcal{V}_n$ that the spaces

$$\mathcal{X}_n := \{u_n \in \mathcal{X}_{l(n)}^1 : u_n \otimes \varphi_n \in \mathcal{V}^{\text{ext}}\}, \quad \langle u_n, v_n \rangle_{\mathcal{X}_n} := \langle u_n \otimes \varphi_n, v_n \otimes \varphi_n \rangle_{\mathcal{V}^{\text{ext}}}, \quad (3.4)$$

equipped with the Hilbert norms $\|u_n\|_{\mathcal{X}_n} := \sqrt{\langle u_n, u_n \rangle_{\mathcal{X}_n}}$ are again Hilbert spaces, and every $u^{\text{ext}} \in \mathcal{V}^{\text{ext}}$ has a unique representation of the form

$$u^{\text{ext}} = \sum_{n \in \mathbb{N}} u_n \otimes \varphi_n, \quad \|u^{\text{ext}}\|_{\mathcal{V}^{\text{ext}}}^2 = \sum_{n \in \mathbb{N}} \|u_n\|_{\mathcal{X}_n}^2, \quad u_n \in \mathcal{X}_n. \quad (3.5)$$

We define the sesquilinear forms $s_n : \mathcal{X}_n \times \mathcal{X}_n \rightarrow \mathbb{C}$ by

$$s_n(u, v) := s(u \otimes \varphi_n, v \otimes \varphi_n).$$

If $v^{\text{ext}} = \sum_{n \in \mathbb{N}} v_n \otimes \varphi_n$, we have

$$s^{\text{ext}}(u^{\text{ext}}, v^{\text{ext}}) = \sum_{n \in \mathbb{N}} s_n(u_n, v_n)$$

due to the assumed orthogonality of the spaces \mathcal{V}_n w.r.t. s^{ext} .

Verification for (3.2): Let as in the introduction $\{\varphi_n : n \in \mathbb{N}\} \subset H_0^1(\tilde{\Gamma}) = \mathcal{Y}^2$ be the complete orthogonal set of eigenfunctions to $-\Delta$, i.e. $-\Delta \varphi_n = \lambda_n \varphi_n$ with $\lambda_n \geq 0$. Since $\{\varphi_n : n \in \mathbb{N}\}$ is also a complete orthogonal set in $H_0^{1/2}(\tilde{\Gamma}) \sim \mathcal{Z}$ and $L^2(\tilde{\Gamma}) = \mathcal{Y}^1$, the orthogonality assumptions are easy to check, $\dim \text{tr}_+(\mathcal{V}_n) = \dim \text{span}\{\varphi_n\} = 1$, and property 3 of Ass. B holds. We have

$$\begin{aligned} \|u\|_{\mathcal{X}_n}^2 &= \|u'\|_{L^2}^2 + (\lambda_n + 2)\|u\|_{L^2}^2, \\ s_n(u, v) &= \langle u', v' \rangle_{L^2} + (\lambda_n - \kappa^2) \langle u, v \rangle_{L^2}. \end{aligned} \quad (3.6)$$

Assumption C: boundedness and coercivity. *There exists a constant $M \in \mathbb{N}$ (later on the number of guided modes), a stability constant $C_s > 0$, a coercivity constant $\alpha > 0$ and rotations $\theta_1, \dots, \theta_M \in \{z \in \mathbb{C} : |z| = 1\}$ such that*

$$|s_n(u_n, v_n)| \leq C_s \|u_n\|_{\mathcal{X}_n} \|v_n\|_{\mathcal{X}_n}, \quad n \in \mathbb{N} \quad (3.7a)$$

$$\Re(\theta_n s_n(u_n, u_n)) \geq \alpha \|u_n\|_{\mathcal{X}_n}^2, \quad n = 1, \dots, M \quad (3.7b)$$

$$\Re(s_n(u_n, u_n)) \geq \alpha \|u_n\|_{\mathcal{X}_n}^2, \quad n > M \quad (3.7c)$$

for all $u_n, v_n \in \mathcal{X}_n$. Moreover, there exists a compact linear operator $K : \mathcal{V}^{\text{int}} \rightarrow \mathcal{V}^{\text{int}}$ such that

$$\Re s^{\text{int}}(u^{\text{int}}, u^{\text{int}}) + \Re \langle K u^{\text{int}}, u^{\text{int}} \rangle_{\mathcal{V}^{\text{int}}} \geq \alpha \|u^{\text{int}}\|^2 \quad \text{for all } u^{\text{int}} \in \mathcal{V}^{\text{int}}. \quad (3.8)$$

It is essential that the constants C_s and α do not depend on n . Due to (3.8), s^{int} is coercive up to a compact perturbation. In our application (PML or HSM formulation for Helmholtz waveguide problems) s^{ext} is neither coercive nor coercive up to a compact perturbation since guided and evanescent modes must be treated differently. This requires the use of \mathcal{S} -coercivity in our analysis. To deal with the coupling to the interior domain, we have to assume that M (the number of guided modes) is finite.

Verification for (3.2): Here $M = 0$, and due to (3.6) assumption (3.7a) holds true with $C_s = 1$, (3.7b) is empty, and (3.7c) holds true with $\alpha = (\lambda_1 - \kappa^2)/(\lambda_1 + 2)$, which is positive due to (3.1).

(3.8) holds true with $K = (\kappa^2 + 1)J^*J$ where $J : \mathcal{V}^{\text{int}} \hookrightarrow L^2(\Omega)$ is the embedding operator, which is compact.

Assumption D: discrete subspaces. We consider families of finite dimensional nested subspaces $\mathcal{V}_h^{\text{int}} \subset \mathcal{V}^{\text{int}}$ and $\mathcal{B}_{h,l} \subset \mathcal{B}_l^2$, which are decreasing in a parameter $h > 0$, and a family of nested subspaces $\mathcal{X}_{N,l} \subset \mathcal{X}_l^2$, which are increasing in a parameter $N \in \mathbb{N}$ such that $\bigcup_{h>0} \mathcal{V}_h^{\text{int}} \subset \mathcal{V}^{\text{int}}$, $\bigcup_{N \in \mathbb{N}} \mathcal{X}_{N,l} \subset \mathcal{X}_l^2$, and $\bigcup_{h>0} \mathcal{B}_{h,l} \subset \mathcal{B}_l^2$ are dense for $l = 1, \dots, L$. Assume that

$$\mathcal{V}_{h,N}^{\text{ext}} \subset \mathcal{V}^{\text{ext}} \quad \text{and} \quad \text{tr}_+(\mathcal{V}_{h,N}^{\text{ext}}) = \text{tr}_-(\mathcal{V}_h^{\text{int}}) \quad (3.9)$$

with $\mathcal{V}_{h,N}^{\text{ext}} := \bigoplus_{l=1}^L \mathcal{X}_{N,l} \otimes \mathcal{B}_{h,l}$ and set

$$\mathcal{V}_{h,N} := \left\{ \begin{pmatrix} u^{\text{int}} \\ u^{\text{ext}} \end{pmatrix} \in \mathcal{V}_h^{\text{int}} \oplus \mathcal{V}_{h,N}^{\text{ext}} : \text{tr}_- u^{\text{int}} = \text{tr}_+ u^{\text{ext}} \right\}.$$

Finally, assume there exist operators $\text{tr}_-^\dagger \in L(\mathcal{Z}, \mathcal{V}^{\text{int}})$ and $\text{tr}_{h,-}^\dagger \in L(\mathcal{Z}, \mathcal{V}_h^{\text{int}})$ such that $\text{tr}_- \text{tr}_-^\dagger = \text{I}_{\mathcal{Z}}$, $\text{tr}_- \text{tr}_{h,-}^\dagger \text{tr}_- u_h^{\text{int}} = \text{tr}_- u_h^{\text{int}}$ for all $u_h^{\text{int}} \in \mathcal{V}_h^{\text{int}}$ and

$$\lim_{h \rightarrow 0} \|\text{tr}_-^\dagger g - \text{tr}_{h,-}^\dagger g\|_{\mathcal{V}^{\text{int}}} = 0 \quad \text{for all } g \in \mathcal{Z}. \quad (3.10)$$

The conditions (3.9) obviously ensure that $\mathcal{V}_{h,N} \subset \mathcal{V}$. We emphasize that it is *not* assumed that any of the orthogonal basis functions ϕ_n is contained in any of the subspaces \mathcal{B}_h . The functions ϕ_n are only used in our analysis, but typically not in the numerical algorithms.

Verification for (3.2): We may start with any sequence of finite element spaces $\mathcal{V}_h^{\text{int}} \subset \mathcal{V}^{\text{int}}$ such that the best approximations to any $u^{\text{int}} \in \mathcal{V}^{\text{int}}$ in $\mathcal{V}_h^{\text{int}}$ converge to u^{int} as $h \rightarrow 0$ and for each h some sub-mesh yields an admissible mesh for $\tilde{\Gamma}$. For $\mathcal{V}_{h,N}^{\text{ext}} = \mathcal{X}_N \otimes \mathcal{B}_h$ we set $\mathcal{B}_h := \text{tr}_-(\mathcal{V}_h)$ and define a non-decreasing mapping $\mathbb{N} \ni N \mapsto \rho_N > 0$ such that $\rho_N \rightarrow \infty$ for $N \rightarrow \infty$. Let $\tilde{\mathcal{X}}_N$ be any $H^1((0, \rho_N))$ -conforming finite element space and

$$\mathcal{X}_N := \{v \in H^1((0, \infty)) \mid v|_{(0, \rho_N)} \in \tilde{\mathcal{X}}_N, \quad v|_{[\rho_N, \infty)} \equiv 0\} \subset \mathcal{X}^2.$$

In order to get nested subspaces, \mathcal{X}_{N+1} has to be constructed such that for $v \in \mathcal{X}_{N+1}$ we have $v|_{(0,\rho_N)} \in \mathcal{X}_N$. This can be done by a suitable refinement of the mesh in $[0, \rho_N]$ (h and/or p refinement) and adding new finite elements for $[\rho_N, \rho_{N+1}]$.

Then $\mathcal{X}_N \otimes \mathcal{Y}_h$ is a finite element space of tensor product finite elements. The continuous right inverse tr_-^\dagger can be constructed by considering the boundary value problem

$$\begin{aligned} -\Delta v + v &= 0 & \text{in } \Omega_{\text{int}}, \\ v &= 0 & \text{on } \partial\Omega_{\text{int}} \setminus \Gamma, \\ v &= g & \text{on } \Gamma, \end{aligned}$$

which obviously has a unique weak solution by the Lax-Milgram lemma, and setting $\text{tr}_-^\dagger g := v$. $\text{tr}_{h,-}^\dagger g$ is the finite element approximation to $\text{tr}_-^\dagger g$ in $\mathcal{V}_h^{\text{int}}$, and (3.10) holds true because of the convergence of the finite element method.

Now we are in a position to formulate our main convergence theorem:

Theorem 3.2. *Suppose Assumptions **A**, **B**, **C** and **D** hold true and assume that the variational equation*

$$s\left(\begin{pmatrix} u^{\text{int}} \\ u^{\text{ext}} \end{pmatrix}, \begin{pmatrix} v^{\text{int}} \\ v^{\text{ext}} \end{pmatrix}\right) = F\left(\begin{pmatrix} v^{\text{int}} \\ v^{\text{ext}} \end{pmatrix}\right) \quad \text{for all } \begin{pmatrix} v^{\text{int}} \\ v^{\text{ext}} \end{pmatrix} \in \mathcal{V} \quad (3.11)$$

has at most one solution for all $F \in \mathcal{V}^$. Then:*

1. *Equation (3.11) has a unique solution $u = \begin{pmatrix} u^{\text{int}} \\ u^{\text{ext}} \end{pmatrix} \in \mathcal{V}$ for all $F \in \mathcal{V}^*$, and u depends continuously on F .*
2. *There exist constants $h_0, C > 0$ such that the discrete variational problems*

$$s(u_{h,N}, v_{h,N}) = F(v_{h,N}) \quad \text{for all } v_{h,N} \in \mathcal{V}_{h,N} \quad (3.12)$$

have unique solutions for all $h \leq h_0$ and all $N \in \mathbb{N}$, and

$$\|u - u_{h,N}\|_{\mathcal{V}} \leq C \inf_{w_{h,N} \in \mathcal{V}_{h,N}} \|u - w_{h,N}\|_{\mathcal{V}}. \quad (3.13)$$

Moreover, the right hand side of (3.13) tends to 0 as $h \rightarrow 0$ and $N \rightarrow \infty$ for all $u \in \mathcal{V}$.

Note that Theorem 3.2 involves an assumption $h \leq h_0$, which is already necessary for the interior problem, but no assumption $N \geq N_0$.

Let us assume that the sesquilinear form $s := s_\kappa$ depends on a parameter $\kappa \in \Lambda$ in a subset $\Lambda \subset \mathbb{C}$. We are looking for solutions $(\kappa, u) \in \Lambda \times \mathcal{V} \setminus \{0\}$ to the continuous generalized eigenvalue problem

$$s_\kappa(u, v) = 0 \quad \text{for all } v \in \mathcal{V}. \quad (3.14)$$

These eigenpairs will be approximated by solutions $(\kappa_{h,N}, u_{h,N}) \in \Lambda \times \mathcal{V}_h \setminus \{0\}$ to the discrete eigenvalue problems

$$s_{\kappa_{h,N}}(u_{h,N}, v_{h,N}) = 0 \quad \text{for all } v_{h,N} \in \mathcal{V}_{h,N}. \quad (3.15)$$

Let $\Sigma \subset \Lambda$ denote the set of eigenvalues κ and $\Sigma_{h,N}$ the set of discrete eigenvalues $\kappa_{h,N}$.

Assumption E: eigenproblem setting. Let $\Lambda \subset \mathbb{C}$ be open and assume that the sesquilinear form $s := s_\kappa$ in Assumption A depends on a parameter $\kappa \in \Lambda$. Moreover, suppose that each $\kappa_0 \in \Lambda$ has a neighborhood $\hat{\Lambda}$ in which the vectors φ_n in Assumption B and the quantities C_s, α, θ_n, M and K in Assumption C can be chosen independently of $\kappa \in \hat{\Lambda}$. Finally, assume that s_κ depends holomorphically on $\kappa \in \Lambda$, i.e. for the operator $T_\kappa : \mathcal{V} \rightarrow \mathcal{V}$ defined by $s_\kappa(u, v) = \langle T_\kappa u, v \rangle_{\mathcal{V}}$, $u, v \in \mathcal{V}$ there exist for all $\kappa_0 \in \Lambda$ the derivative $T'_{\kappa_0} := \lim_{\kappa \rightarrow \kappa_0} \frac{1}{\kappa - \kappa_0} (T_\kappa - T_{\kappa_0})$ where the limit exists in the norm of $L(\mathcal{V})$.

Verification for (3.2): If s_κ is defined by the left hand side of (3.2), then it depends holomorphically on κ . Clearly φ_n is independent of κ , $M = 0$ does not depend on κ and θ_n is not needed. If $\min \sigma(-\Delta_1) = \lambda_1$ and for all $\kappa_0 \in \Lambda$ there holds $\Re(\kappa_0^2) < \lambda_1$, then $\alpha = \inf_{\kappa \in \hat{\Lambda}} \Re(\lambda_1 - \kappa^2) / (\lambda_1 + 2)$ is independent of κ_0 as well and positive, if $\hat{\Lambda}$ is compact. In the same way C_s and K can be chosen independently of $\kappa \in \hat{\Lambda}$.

Remark 3.3. Up to now we have not defined a complex square root and therefore κ_n defined in (2.4) for $\kappa > 0$ is not defined for $\kappa \in \mathbb{C} \setminus \mathbb{R}$. We will do this later in Def. 5.3. At this point, we only consider (3.2) and do not care whether the eigenvalues are physically meaningful.

Theorem 3.4. If Assumptions A, B, C, D and E hold true and if there exists a $\kappa \in \Lambda$ such that T_κ is invertible, then $\Sigma \subset \Lambda$ is discrete without accumulation points and

$$\lim_{h \rightarrow 0, N \rightarrow \infty} \text{dist}(\Sigma \cap \Lambda', \Sigma_{h,N} \cap \Lambda') = 0 \quad (3.16)$$

for all compact subsets $\Lambda' \subset \Lambda$. Here the Hausdorff distance of two subsets $A, B \subset \mathbb{C}$ is denoted by $\text{dist}(A, B) := \max\{\sup_{a \in A} \inf_{b \in B} |a - b|, \sup_{b \in B} \inf_{a \in A} |a - b|\}$.

Further convergence results including convergence of eigenvectors (or eigenspaces), multiplicities of eigenvalues, and rates of convergence are intended for future research.

4 Proof of Theorems 3.2 and 3.4

The convergence theory is based on S-coercivity arguments: We are going to construct an isomorphism $S : \mathcal{V} \rightarrow \mathcal{V}$ such that the sesquilinear form $s(S \cdot, \cdot)$ is coercive up to a compact perturbation. Hence, unique solvability of the continuous problem can be shown as usual using the Lax-Milgram Lemma combined with Riesz-Fredholm theory. An important difficulty is the fact that the discrete spaces $\mathcal{V}_{h,N}$ are not invariant under S . In order to overcome this difficulty we will introduce later on a family of operators $S_h : \mathcal{V}_{h,N} \rightarrow \mathcal{V}_{h,N}$ with $\|S - S_h\|_{L(\mathcal{V}_{h,N}, \mathcal{V})} \rightarrow 0$ for $h \rightarrow 0$.

4.1 Construction and properties of the operator S

Using the notation of Ass. B we define in the exterior domain the operator

$$S^{\text{ext}} : \mathcal{V}^{\text{ext}} \rightarrow \mathcal{V}^{\text{ext}}, \quad S^{\text{ext}} u^{\text{ext}} := \sum_{n=1}^M \theta_n u_n^{\text{ext}} \otimes \varphi_n + \sum_{n=M+1}^{\infty} u_n^{\text{ext}} \otimes \varphi_n \quad (4.1)$$

where u^{ext} has the expansion (3.5). Recall, that the rotations θ_n and the constant M were introduced in Ass. C. With the operator S^{ext} we have S-coercivity and boundedness of s^{ext} by Assumption C:

$$\begin{aligned} \Re(s^{\text{ext}}(S^{\text{ext}} u^{\text{ext}}, u^{\text{ext}})) &\geq \alpha \|u^{\text{ext}}\|_{\mathcal{V}^{\text{ext}}}^2 \\ |s^{\text{ext}}(u^{\text{ext}}, v^{\text{ext}})| &\leq C_s \|u^{\text{ext}}\|_{\mathcal{V}^{\text{ext}}} \|v^{\text{ext}}\|_{\mathcal{V}^{\text{ext}}} \end{aligned} \quad (4.2)$$

for all $u^{\text{ext}}, v^{\text{ext}} \in \mathcal{V}^{\text{ext}}$. Note, that S^{ext} has a bounded inverse given by

$$[S^{\text{ext}}]^{-1} u^{\text{ext}} := \sum_{n=1}^M \frac{1}{\theta_n} u_n^{\text{ext}} \otimes \varphi_n + \sum_{n=M+1}^{\infty} u_n^{\text{ext}} \otimes \varphi_n.$$

We need to extend S^{ext} to the whole space \mathcal{V} via the trace space \mathcal{Z} defined in Assumption A. First we define a bounded linear operator $S^{\mathcal{Z}} : \mathcal{Z} \rightarrow \mathcal{Z}$ such that S^{ext} and $S^{\mathcal{Z}}$ intertwine with tr_+ :

$$S^{\mathcal{Z}} \text{tr}_+ = \text{tr}_+ S^{\text{ext}}. \quad (4.3)$$

As $\mathcal{Z} = \bigoplus_{n \in \mathbb{N}} \text{tr}_+(\mathcal{V}_n)$ by Assumption B we have to set $S^{\mathcal{Z}} \psi_n := \theta_n \psi_n$ for all $\psi_n \in \text{tr}_+(\mathcal{V}_n^{\text{ext}})$ and $n \leq M$ and $S^{\mathcal{Z}} \psi_n := \psi_n$ if $n > M$. As for S^{ext} it is easy to see that $S^{\mathcal{Z}}$ has a bounded inverse.

Using $\text{tr}_-^\dagger : \mathcal{Z} \rightarrow \mathcal{V}^{\text{int}}$ defined in Ass. D we can define $S : \mathcal{V} \rightarrow \mathcal{V}$ by

$$S \begin{pmatrix} u^{\text{int}} \\ u^{\text{ext}} \end{pmatrix} := \begin{pmatrix} u^{\text{int}} + \text{tr}_-^\dagger (S^{\mathcal{Z}} - \text{I}) \text{tr}_- u^{\text{int}} \\ S^{\text{ext}} u^{\text{ext}} \end{pmatrix}. \quad (4.4)$$

The image of \mathcal{V} under S is in fact contained in \mathcal{V} since

$$\text{tr}_- u^{\text{int}} + \text{tr}_-^\dagger (S^{\mathcal{Z}} - \text{I}) \text{tr}_- u^{\text{int}} = S^{\mathcal{Z}} \text{tr}_- u^{\text{int}} = S^{\mathcal{Z}} \text{tr}_+ u^{\text{ext}} = \text{tr}_+ S^{\text{ext}} u^{\text{ext}}.$$

S has the bounded inverse

$$S^{-1} \begin{pmatrix} u^{\text{int}} \\ u^{\text{ext}} \end{pmatrix} = \begin{pmatrix} u^{\text{int}} + \text{tr}_-^\dagger ([S^{\mathcal{Z}}]^{-1} - \text{I}) \text{tr}_- u^{\text{int}} \\ [S^{\text{ext}}]^{-1} u^{\text{ext}} \end{pmatrix},$$

which is easily verified using the identity

$$S^{\mathcal{Z}} - \text{I} + [S^{\mathcal{Z}}]^{-1} - \text{I} + (S^{\mathcal{Z}} - \text{I})([S^{\mathcal{Z}}]^{-1} - \text{I}) = 0.$$

4.2 Proof of Theorem 3.2, part 1

With the substitution $\tilde{u} := S^{-1} \begin{pmatrix} u^{\text{int}} \\ u^{\text{ext}} \end{pmatrix}$ the variational equation (3.11) is equivalent to

$$\tilde{s}(\tilde{u}, v) = F(v), \quad \tilde{s}(\tilde{u}, v) := s(S\tilde{u}, v)$$

for all $v = (v^{\text{int}}, v^{\text{ext}}) \in \mathcal{V}$. Since the homogeneous equation is assumed to be uniquely solvable, the bounded linear operator $A : \mathcal{V} \rightarrow \mathcal{V}$ defined by $\tilde{s}(u, v) = \langle Au, v \rangle_{\mathcal{V}}$ for all $u, v \in \mathcal{V}$ is injective. Due to (3.8) and (4.2) we have

$$\begin{aligned} \Re \tilde{s} \left(\begin{pmatrix} u^{\text{int}} \\ u^{\text{ext}} \end{pmatrix}, \begin{pmatrix} u^{\text{int}} \\ u^{\text{ext}} \end{pmatrix} \right) + \Re \left\langle (K - \tilde{K}) u^{\text{int}}, u^{\text{int}} \right\rangle_{\mathcal{V}^{\text{int}}} &\geq \alpha \left\| \begin{pmatrix} u^{\text{int}} \\ u^{\text{ext}} \end{pmatrix} \right\|_{\mathcal{V}}^2, \\ \tilde{K} &:= \text{tr}_-^\dagger (S^{\mathcal{Z}} - \text{I}) \text{tr}_- \end{aligned} \quad (4.5)$$

for all $\begin{pmatrix} u^{\text{int}} \\ u^{\text{ext}} \end{pmatrix} \in \mathcal{V}$. It follows from the Lax-Milgram lemma that $A + \begin{pmatrix} K-\tilde{K} & 0 \\ 0 & 0 \end{pmatrix}$ is boundedly invertible. Since $\dim(\mathcal{S} - \mathbf{I})(\mathcal{Z}) < \infty$, the operator \tilde{K} is compact. Together with the injectivity of A it follows from Riesz-Fredholm theory that A has a bounded inverse. This implies the first assertion.

4.3 Proof of Theorem 3.2, part 2

We first show sufficient conditions for discrete inf-sup stability for general S -coercive problems:

Lemma 4.1. *Let \mathcal{V} be any complex Hilbert space and $s : \mathcal{V} \times \mathcal{V} \rightarrow \mathbb{C}$ a bounded sesquilinear form and $S : \mathcal{V} \rightarrow \mathcal{V}$ a bounded linear operator. Moreover, let $\mathcal{V}_h \subset \mathcal{V}$ be a series of closed subspaces, $P_h : \mathcal{V} \rightarrow \mathcal{V}_h$ the orthogonal projections. Then*

$$\inf_{\substack{v_h \in \mathcal{V}_h \\ v_h \neq 0}} \sup_{\substack{u_h \in \mathcal{V}_h \\ u_h \neq 0}} \frac{|s(u_h, v_h)|}{\|u_h\|_{\mathcal{V}} \|v_h\|_{\mathcal{V}}} \geq \frac{1}{\|S\|} \left(\inf_{\substack{v_h \in \mathcal{V}_h \\ v_h \neq 0}} \sup_{\substack{u_h \in \mathcal{V}_h \\ u_h \neq 0}} \frac{|s(Su_h, v_h)|}{\|u_h\|_{\mathcal{V}} \|v_h\|_{\mathcal{V}}} - \|s\| \|(I - P_h)SP_h\|_{L(\mathcal{V})} \right).$$

In particular, if s is S -coercive, i.e. there exists a constant $\tilde{\alpha} > 0$, such that $s(Su, u) \geq \tilde{\alpha}\|u\|_{\mathcal{V}}^2$ and if

$$\lim_{h \rightarrow 0} \|(I - P_h)SP_h\|_{L(\mathcal{V})} = 0, \quad (4.6)$$

then s is discretely inf-sup stable for sufficiently small $h > 0$ with constants independent of h .

Proof. For all $v_h \in \mathcal{V}_h$ we have

$$\begin{aligned} \sup_{\substack{u_h \in \mathcal{V}_h \\ u_h \neq 0}} \frac{|s(u_h, v_h)|}{\|u_h\|_{\mathcal{V}}} &\geq \sup_{\substack{u_h \in \mathcal{V}_h \\ P_h Su_h \neq 0}} \frac{|s(Su_h, v_h) - s((P_h - I)SP_h u_h, v_h)|}{\|P_h Su_h\|_{\mathcal{V}}} \\ &\geq \frac{1}{\|S\|} \left(\sup_{\substack{u_h \in \mathcal{V}_h \\ u_h \neq 0}} \frac{|s(Su_h, v_h)|}{\|u_h\|_{\mathcal{V}}} - \|s\| \|(P_h - I)SP_h\|_{L(\mathcal{V})} \|v_h\|_{\mathcal{V}} \right). \end{aligned}$$

The proposition follows by dividing this inequality by $\|v_h\|_{\mathcal{V}}$ and taking the infimum over all $v_h \in \mathcal{V}_h$. \square

Now let us verify condition (4.6):

Lemma 4.2. *Suppose Assumptions A-D hold true, and let $P_{h,N} : \mathcal{V} \rightarrow \mathcal{V}_{h,N}$ denote the orthogonal projections. Then*

$$\lim_{h \rightarrow 0} \sup_{N \in \mathbb{N}} \|(I - P_{h,N})SP_{h,N}\|_{L(\mathcal{V})} = 0.$$

Proof. Recall, that the discrete spaces $\mathcal{V}_{h,N}$ and the corresponding quantities like the discrete trace operators $\text{tr}_{h,-}^{\dagger} : \mathcal{Z} \rightarrow \mathcal{V}_h^{\text{int}}$ as well as the $\mathcal{V}_{h,N}^{\text{ext}} = \bigoplus_{l=1}^L \mathcal{X}_{N,l} \otimes \mathcal{Y}_{h,l}$ with $\mathcal{X}_{N,l} \subset \mathcal{X}_l^2$ and $\mathcal{Y}_{h,l} \subset \mathcal{Y}_l^2$ were introduced in Ass. D.

Since $P_{h,N} : \mathcal{V} \rightarrow \mathcal{V}_{h,N}$ denotes the orthogonal projection, it holds

$$\|(I - P_{h,N})S P_{h,N}\|_{L(\mathcal{V})} = \sup_{\substack{u \in \mathcal{V}_{h,N} \\ u \neq 0}} \frac{\|(I - P_{h,N})Su\|_{\mathcal{V}}}{\|u\|_{\mathcal{V}}} = \sup_{\substack{u \in \mathcal{V}_{h,N} \\ u \neq 0}} \inf_{v \in \mathcal{V}_{h,N}} \frac{\|Su - v\|_{\mathcal{V}}}{\|u\|_{\mathcal{V}}}. \quad (4.7)$$

To estimate the right hand side of this equation choose $u = \begin{pmatrix} u^{\text{int}} \\ u^{\text{ext}} \end{pmatrix} \in \mathcal{V}_{h,N}$. In the unique expansion $u^{\text{ext}} = \sum_{n \in \mathbb{N}} u_n \otimes \varphi_n$ (see (3.5)) all u_n belong to \mathcal{X}_N . By definition of S in (4.1) we have

$$S^{\text{ext}} u^{\text{ext}} = u^{\text{ext}} + \sum_{n=1}^M (\theta_n - 1) u_n \otimes \varphi_n.$$

We set $S_h^{\text{ext}} u^{\text{ext}} := u^{\text{ext}} + \sum_{n=1}^M (\theta_n - 1) u_n \otimes P_h^{\mathcal{Y}} \varphi_n$ with the orthogonal projection $P_h^{\mathcal{Y}} : \bigoplus_l \mathcal{Y}_l^2 \rightarrow \bigoplus_l \mathcal{Y}_{h,l}$. As $S_h^{\text{ext}} u^{\text{ext}} \in \mathcal{V}_{h,N}^{\text{ext}}$, we can set $v^{\text{ext}} := S_h^{\text{ext}} u^{\text{ext}}$ later.

Due to Ass. B there exists for $n \in \mathbb{N}$ a $l(n) \in \{1, \dots, L\}$ such that for $\varphi_n = (\varphi_n^{(1)}, \dots, \varphi_n^{(L)})$ it holds $\varphi_n^{(j)} = 0$ for $j \neq l(n)$. Using the definition of $\|\cdot\|_{\mathcal{V}^{\text{ext}}}$ in (3.3) we have

$$\begin{aligned} \|S^{\text{ext}} u^{\text{ext}} - S_h^{\text{ext}} u^{\text{ext}}\|_{\mathcal{V}^{\text{ext}}} &= \left\| \sum_{n=1}^M (\theta_n - 1) u_n \otimes (\varphi_n - P_h^{\mathcal{Y}} \varphi_n) \right\|_{\mathcal{V}^{\text{ext}}} \\ &\leq 2 \sum_{n=1}^M \|u_n \otimes (\varphi_n - P_h^{\mathcal{Y}} \varphi_n)\|_{\mathcal{V}^{\text{ext}}} \\ &= 2 \sum_{n=1}^M \left(\|u_n\|_{\mathcal{X}_{l(n)}^2}^2 \|\varphi_n^{(l(n))} - P_h^{\mathcal{Y}_{l(n)}^2} \varphi_n^{(l(n))}\|_{\mathcal{Y}_{l(n)}^1}^2 + \|u_n\|_{\mathcal{X}_{l(n)}^1}^2 \|\varphi_n^{(l(n))} - P_h^{\mathcal{Y}_{l(n)}^2} \varphi_n^{(l(n))}\|_{\mathcal{Y}_{l(n)}^2}^2 \right)^{1/2} \\ &\leq 2C_{M,h} \sum_{n=1}^M \left(\|u_n\|_{\mathcal{X}_{l(n)}^2}^2 \|\varphi_n^{(l(n))}\|_{\mathcal{Y}_{l(n)}^1}^2 + \|u_n\|_{\mathcal{X}_{l(n)}^1}^2 \|\varphi_n^{(l(n))}\|_{\mathcal{Y}_{l(n)}^2}^2 \right)^{1/2} \\ &= 2C_{M,h} \sum_{n=1}^M \|u_n \otimes \varphi_n\|_{\mathcal{V}^{\text{ext}}} \leq 2C_{M,h} \sqrt{M} \left(\sum_{n=1}^M \|u_n \otimes \varphi_n\|_{\mathcal{V}^{\text{ext}}}^2 \right)^{1/2} \leq 2C_{M,h} \sqrt{M} \|u\|_{\mathcal{V}^{\text{ext}}} \end{aligned}$$

with

$$C_{M,h} := \max_{n=1 \dots M} \max \left\{ \frac{\|\varphi_n^{(l(n))} - P_h^{\mathcal{Y}_{l(n)}^2} \varphi_n^{(l(n))}\|_{\mathcal{Y}_{l(n)}^1}}{\|\varphi_n^{(l(n))}\|_{\mathcal{Y}_{l(n)}^1}}, \frac{\|\varphi_n^{(l(n))} - P_h^{\mathcal{Y}_{l(n)}^2} \varphi_n^{(l(n))}\|_{\mathcal{Y}_{l(n)}^2}}{\|\varphi_n^{(l(n))}\|_{\mathcal{Y}_{l(n)}^2}} \right\}.$$

Due to the density $\bigcup_h \mathcal{Y}_{h,l} \subset \mathcal{Y}_l^2$, the finiteness of M and the continuity of the embeddings $\mathcal{Y}_l^2 \hookrightarrow \mathcal{Y}_l^1$, we have $\lim_{h \rightarrow 0} C_{M,h} = 0$, i.e.

$$\lim_{h \rightarrow 0} \sup_{N \in \mathbb{N}} \|S^{\text{ext}} - S_h^{\text{ext}}\|_{L(\mathcal{V}_{h,N}^{\text{ext}}, \mathcal{V}^{\text{ext}})} = 0. \quad (4.8)$$

We define $S_h : \mathcal{V}_{h,N} \rightarrow \mathcal{V}_{h,N}$ by

$$S_h \begin{pmatrix} u^{\text{int}} \\ u^{\text{ext}} \end{pmatrix} := \begin{pmatrix} u^{\text{int}} + \text{tr}_{h,-}^{\dagger} (\text{tr}_+ S_h^{\text{ext}} u^{\text{ext}} - \text{tr}_- u^{\text{int}}) \\ S_h^{\text{ext}} u^{\text{ext}} \end{pmatrix}.$$

Then using $\text{tr}_- u^{\text{int}} = \text{tr}_+ u^{\text{ext}}$ we have

$$\begin{aligned} \left[(S - S_h) \begin{pmatrix} u^{\text{int}} \\ u^{\text{ext}} \end{pmatrix} \right]^{\text{int}} &= \left(\text{tr}_-^\dagger \text{tr}_+ S^{\text{ext}} - \text{tr}_{h,-}^\dagger \text{tr}_+ S_h^{\text{ext}} \right) u^{\text{ext}} + \left(\text{tr}_{h,-}^\dagger - \text{tr}_-^\dagger \right) \text{tr}_- u^{\text{int}} \\ &= \left(\text{tr}_-^\dagger - \text{tr}_{h,-}^\dagger \right) \text{tr}_+ (S^{\text{ext}} - I) u^{\text{ext}} + \text{tr}_{h,-}^\dagger \text{tr}_+ (S^{\text{ext}} - S_h^{\text{ext}}) u^{\text{ext}} \end{aligned}$$

Since the range of $\text{tr}_+ (S^{\text{ext}} - I)$ is finite dimensional and $\text{tr}_-^\dagger - \text{tr}_{h,-}^\dagger$ converges point wise to 0 (3.10), we have $\lim_{h \rightarrow 0} \|(\text{tr}_-^\dagger - \text{tr}_{h,-}^\dagger) \text{tr}_+ (S^{\text{ext}} - I)\|_{L(\mathcal{V}^{\text{ext}}, \mathcal{V}^{\text{int}})} = 0$. Moreover, by the uniform boundedness principle $\sup_{h > 0} \|\text{tr}_{h,-}^\dagger\|_{L(\mathcal{X}, \mathcal{V}^{\text{int}})} < \infty$. Together with (4.8) this implies

$$\lim_{h \rightarrow 0} \sup_{N \in \mathbb{N}} \left\| [S - S_h]^{\text{int}} \right\|_{L(\mathcal{V}_{h,N}, \mathcal{V}^{\text{int}})} = 0. \quad (4.9)$$

Setting $v := S_h u$ in (4.7) and combining (4.8) and (4.9) we obtain

$$\sup_{N \in \mathbb{N}} \|(I - P_{h,N}) S P_{h,N}\|_{L(\mathcal{V})} \leq \sup_{N \in \mathbb{N}} \|S - S_h\|_{L(\mathcal{V}_{h,N}, \mathcal{V})} \xrightarrow{h \rightarrow 0} 0.$$

□

Lemma 4.3. *Under Assumptions A-D $\bigcup_{h>0, N \in \mathbb{N}} \mathcal{V}_{h,N} \subset \mathcal{V}$ is dense.*

Proof. Assume that $\langle w, u_{h,N} \rangle = 0$ for all $u \in \mathcal{V}_{h,N}$ and all h, N for some $w \in \mathcal{V}$. In particular

$$0 = \left\langle w^{\text{int}}, \text{tr}_{h,-}^\dagger \text{tr}_+ (v_N \otimes \psi_h) \right\rangle_{\mathcal{V}^{\text{int}}} + \left\langle w^{\text{ext}}, v_N \otimes \psi_h \right\rangle_{\mathcal{V}^{\text{ext}}}$$

for all $v_N \in \mathcal{X}_N$ and $\psi_h \in \mathcal{Y}_h$. Due to the form of the inner product of \mathcal{V}^{ext} , the assumptions on \mathcal{X}_N and \mathcal{Y}_h and the point wise convergence of $\text{tr}_{h,-}^\dagger$, we have

$$0 = \left\langle w^{\text{int}}, \text{tr}_-^\dagger \text{tr}_+ (u^{\text{ext}}) \right\rangle_{\mathcal{V}^{\text{int}}} + \left\langle w^{\text{ext}}, u^{\text{ext}} \right\rangle_{\mathcal{V}^{\text{ext}}} \quad (4.10)$$

first for all u^{ext} of the form $u^{\text{ext}} = v \otimes \psi$ with $v \in \mathcal{X}^2$ and $\psi \in \mathcal{Y}^2$ and then by density of $\mathcal{X}^2 \subset \mathcal{X}^1$ and $\mathcal{Y}^2 \subset \mathcal{Y}^1$ for all $u^{\text{ext}} \in \mathcal{V}^{\text{ext}}$.

For a given $u := (u^{\text{int}}, u^{\text{ext}})^\top \in \mathcal{V}$ we obtain with (4.10), $\text{tr}_- u^{\text{int}} = \text{tr}_+ u^{\text{ext}}$ and the density assumption on $\mathcal{V}_h^{\text{int}}$

$$\langle w, u \rangle_{\mathcal{V}} = \left\langle w^{\text{int}}, u^{\text{int}} - \text{tr}_-^\dagger \text{tr}_- u^{\text{int}} \right\rangle_{\mathcal{V}^{\text{int}}} = 0.$$

This shows that $w = 0$. Hence the orthogonal complement of $\bigcup_{h,N} \mathcal{V}_{h,N}$ is $\{0\}$, i.e. this space is dense in \mathcal{V} . □

We can now complete the proof of the second part of Theorem 3.2 as follows: Due to (4.5) and Lemmas 4.1 and 4.2 the discrete inf-sup constants of the variational problems

$$s(u_{h,N}, v_{h,N}) + \left\langle (K - \tilde{K}) u_h^{\text{int}}, v_h^{\text{int}} \right\rangle_{\mathcal{V}^{\text{int}}} = F(v_{h,N}), \quad v_{h,N} = \begin{pmatrix} v_h^{\text{int}} \\ v_{h,N}^{\text{ext}} \end{pmatrix} \in \mathcal{V}_{h,N} \quad (4.11)$$

are uniformly bounded away from 0 for $h \leq h_0$. Therefore, these variational equations have unique solutions $u_{h,N} \in \mathcal{V}_{h,N}$ for all $h \leq h_0$, and together with the density lemma 4.3 it follows that the Galerkin method (4.11) converges, and the error bound (3.13) holds true for this modified problem (see e.g. [17, Theorems 13.6]). Since $K - \tilde{K}$ is compact the Galerkin method (3.12) for the original problem (3.11) converges as well with error bound (3.13) (see e.g. [17, Theorems 13.6 and 13.7]).

4.4 Proof of Theorem 3.4

For the following we need in addition to Ass. A-D the Ass. E for the eigenvalue setting. Recall, that Σ denotes the set of eigenvalues κ of $s_\kappa(u, v) = 0$, $v \in \mathcal{V}$, with eigenfunction $u \in \mathcal{V} \setminus \{0\}$. Moreover, if there exists a $\kappa \in \Lambda$ such that the operator $T_\kappa : \mathcal{V} \rightarrow \mathcal{V}$ defined by $s_\kappa(u, v) = \langle T_\kappa u, v \rangle_{\mathcal{V}}$, $u, v \in \mathcal{V}$, is invertible, then Σ is discrete without accumulation points by analytic Fredholm theory (see e.g. [7, Part III, Cor. XI.8.4]). Note, that we have shown in Sec. 4.2, that T_κ is a Fredholm operator for all $\kappa \in \Lambda$.

As opposed to some other eigenvalue convergence results (see e.g. [8, Chapter 11]) some complications arise since we do not have a compact embedding assumption in the exterior domain. (Recall that e.g. $H^1(\Omega_{\text{ext}}) \hookrightarrow L^2(\Omega_{\text{ext}})$ is not compact due to the unboundedness of Ω_{ext} .) We could use as in [28, Sec. 4] the abstract framework of [15]. Nevertheless, in order to be self-consistent we present here the proofs in our framework.

Let us define

$$\beta(\kappa) := \inf_{\substack{u \in \mathcal{V} \\ u \neq 0}} \sup_{\substack{v \in \mathcal{V} \\ v \neq 0}} \frac{|s_\kappa(u, v)|}{\|u\|_{\mathcal{V}} \|v\|_{\mathcal{V}}}, \quad \beta_{h,N}(\kappa) := \inf_{\substack{u \in \mathcal{V}_{h,N} \\ u \neq 0}} \sup_{\substack{v \in \mathcal{V}_{h,N} \\ v \neq 0}} \frac{|s_\kappa(u, v)|}{\|u\|_{\mathcal{V}} \|v\|_{\mathcal{V}}}.$$

As a consequence of Theorem 3.2 the operators T_κ have a bounded inverse for all $\kappa \in \Lambda \setminus \Sigma$, and by a Neumann series argument the mapping $\kappa \mapsto T_\kappa^{-1}$ is holomorphic on $\Lambda \setminus \Sigma$. As $\beta(\kappa) = \|T_\kappa^{-1}\|^{-1}$ and $\|s_\kappa\| = \|T_\kappa\|_{L(\mathcal{V})}$, we have

$$\beta \text{ is continuous on } \Lambda \setminus \Sigma \quad (4.12)$$

$$C_{\Lambda'} := \sup\{\|s_\kappa\| \mid \kappa \in \Lambda'\} \text{ is finite} \quad (4.13)$$

for all compact $\Lambda' \subset \Lambda$.

Lemma 4.4. *Under the assumptions of Theorem 3.4 suppose that $\inf\{\beta(\kappa) : \kappa \in \hat{\Lambda}\} > 0$ for some compact subset $\hat{\Lambda} \subset \Lambda$ as in Assumption E. Then there exist constants $\rho, h_0, N_0 > 0$ such that*

$$\beta_{h,N}(\kappa) \geq \rho \quad \text{for all } h \leq h_0, N \geq N_0, \kappa \in \hat{\Lambda}.$$

Proof. Note that by Assumption E the operator S is independent of κ . From Lemmas 4.1 and 4.2 we deduce that there exists $\eta(h, N)$ independent of $\kappa \in \hat{\Lambda}$ with $\eta(h, N) \rightarrow 0$ for $h \rightarrow 0$ and $N \rightarrow \infty$ such that

$$\beta_{h,N}(\kappa) \geq \frac{1}{\|S\|} \inf_{\substack{u \in \mathcal{V}_{h,N} \\ u \neq 0}} \sup_{\substack{v \in \mathcal{V}_{h,N} \\ v \neq 0}} \frac{|s_\kappa(Su, v)|}{\|u\|_{\mathcal{V}} \|v\|_{\mathcal{V}}} - \eta(h, N). \quad (4.14)$$

Therefore, the proof is done if we can show the assertion for $\tilde{s}_\kappa := s_\kappa(\mathbf{S}\bullet, \bullet)$ and

$$\tilde{\beta}_{h,N}(\kappa) := \inf_{\substack{u \in \mathcal{V}_{h,N} \\ u \neq 0}} \sup_{\substack{v \in \mathcal{V}_{h,N} \\ v \neq 0}} \frac{|\tilde{s}_\kappa(u, v)|}{\|u\|_{\mathcal{V}} \|v\|_{\mathcal{V}}}. \quad (4.15)$$

Equivalently, if we define $\tilde{T}(\kappa) : \mathcal{V} \rightarrow \mathcal{V}$ by $\tilde{s}_\kappa(u, v) = \langle \tilde{T}(\kappa)u, v \rangle$ for all $u, v \in \mathcal{V}$, and $\tilde{T}_{h,N}(\kappa) := P_{h,N}\tilde{T}(\kappa) : \mathcal{V}_{h,N} \rightarrow \mathcal{V}_{h,N}$, we have to show due to $\tilde{\beta}_{h,N}(\kappa) = \|\tilde{T}_{h,N}(\kappa)^{-1}\|^{-1}$, that there exist $h_0, N_0, \rho > 0$ independent of $\kappa \in \hat{\Lambda}$ such that $\|\tilde{T}_{h,N}(\kappa)^{-1}\| \leq 1/\rho$ for all $h \leq h_0, N \geq N_0$. If $\hat{\Lambda}$ is a singleton, the assertion follows from [17, Theorem 13.7(2)]. For compact $\hat{\Lambda}$ we can argue similarly keeping track of dependencies on $\kappa \in \hat{\Lambda}$.

Using $\hat{K} := \begin{pmatrix} K - \hat{K} & 0 \\ 0 & 0 \end{pmatrix}$ as in Sec. 4.2, $A(\kappa) := \tilde{T}(\kappa) + \hat{K}$ and $A_{h,N}(\kappa) := P_{h,N}A(\kappa)$ we can factorize

$$\tilde{T}_{h,N}(\kappa) = P_{h,N}\tilde{T}(\kappa) = A_{h,N}(\kappa) (\mathbf{I} - A_{h,N}(\kappa)^{-1}P_{h,N}\hat{K}). \quad (4.16)$$

By Assumptions A-E we have

$$\begin{aligned} \|A(\kappa)\| &\leq C_{\hat{\Lambda}}\|\mathbf{S}\| + \|\hat{K}\|, & \|A(\kappa)^{-1}\| &\leq \alpha^{-1}, \\ \|A_{h,N}(\kappa)^{-1}\| &\leq \alpha^{-1}, & \|\tilde{T}(\kappa)^{-1}\| &= \|\tilde{\beta}(\kappa)^{-1}\| \leq \|\mathbf{S}^{-1}\|/\rho, \\ \|(\mathbf{I} - A(\kappa)^{-1}\hat{K})^{-1}\| &\leq \|A(\kappa)\| \|\tilde{T}(\kappa)^{-1}\| \leq \rho^{-1} \|\mathbf{S}\| \|\mathbf{S}^{-1}\| (C_{\hat{\Lambda}} + \|\hat{K}\|) \end{aligned}$$

for all $\kappa \in \hat{\Lambda}$. By Galerkin orthogonality and coercivity we have

$$\|A_{h,N}(\kappa)^{-1}P_{h,N}f - A(\kappa)^{-1}f\| \leq \frac{\|A(\kappa)\|}{\alpha} \inf_{v \in \mathcal{V}_{h,N}} \|A(\kappa)^{-1}f - v\|_{\mathcal{V}}, \quad \text{for all } f \in \mathcal{V}.$$

Therefore by density of $\bigcup_{h,N} \mathcal{V}_{h,N} \subset \mathcal{V}$, compactness of $\hat{\Lambda}$, and continuity of $\kappa \mapsto A(\kappa)^{-1}$ we have

$$\lim_{h \rightarrow 0, N \rightarrow \infty} \sup_{\kappa \in \hat{\Lambda}} \|A_{h,N}(\kappa)^{-1}P_{h,N}f - A(\kappa)^{-1}f\| = 0 \quad \text{for all } f \in \mathcal{V}. \quad (4.17)$$

We will show that this implies

$$\lim_{h \rightarrow 0, N \rightarrow \infty} \sup_{\kappa \in \hat{\Lambda}} \|(A(\kappa)^{-1} - A_{h,N}(\kappa)^{-1}P_{h,N})\hat{K}\|_{L(\mathcal{V})} = 0. \quad (4.18)$$

In fact, for given $\varepsilon > 0$ the relatively compact set $U := \{\hat{K}f \mid \|f\| \leq 1\}$ can be covered by a finite number of balls $B_r(f_m)$, $m = 1, \dots, M(\varepsilon)$ with radius $r := \varepsilon/3 \sup_{\kappa \in \hat{\Lambda}} \|A(\kappa)\|$. Due to (4.17) there exist $h_0, N_0 > 0$ such that $\|A_{h,N}(\kappa)^{-1}P_{h,N}f_j - A(\kappa)^{-1}f_j\| \leq \varepsilon/3$ for all $j = 1, \dots, M(\varepsilon)$, $h \leq h_0, N \geq N_0$ and $\kappa \in \hat{\Lambda}$. Since all $f \in U$ are contained in some ball $B_r(f_j)$, we have

$$\begin{aligned} \|A_{h,N}(\kappa)^{-1}P_{h,N}f - A(\kappa)^{-1}f\| &\leq \|A_{h,N}(\kappa)^{-1}P_{h,N}(f - f_j)\| \\ &+ \|A_{h,N}(\kappa)^{-1}P_{h,N}f_j - A(\kappa)^{-1}f_j\| + \|A(\kappa)^{-1}(f_j - f)\| \leq 2(C_{\hat{\Lambda}}\|\mathbf{S}\| + \|\hat{K}\|)r + \frac{\varepsilon}{3} = \varepsilon \end{aligned}$$

completing the proof of (4.18). Hence by a Neumann series argument (see [17, Theorem 10.1]) we have

$$\|(\mathbf{I} - A_{h,N}(\kappa)^{-1} P_{h,N} \hat{K})^{-1}\| \leq \frac{\|(\mathbf{I} - A(\kappa)^{-1} \hat{K})^{-1}\|}{1 - \|(\mathbf{I} - A(\kappa)^{-1} \hat{K})^{-1} (A(\kappa)^{-1} \hat{K} - A_{h,N}(\kappa)^{-1} P_{h,N} \hat{K})\|},$$

if the denominator is positive. By (4.18) there are $h_0, N_0 > 0$ such that the denominator is $\geq \frac{1}{2}$ for all $h \leq h_0$ and $N \geq N_0$. In view of (4.16) this implies uniform boundedness of $\|\tilde{T}_{h,N}(\kappa)^{-1}\|$ in h, N , and κ . \square

Proposition 4.5. *Under the assumptions of Theorem 3.4 the following holds true:*

1. *If there exists a sequence $(\kappa_{h,N}) \subset \Lambda'$ of discrete eigenvalues to (3.15) converging to $\kappa_0 \in \Lambda'$ as $h \rightarrow 0$ and $N \rightarrow \infty$, then $\kappa_0 \in \Sigma$.*
2. *For each $\kappa_0 \in \Sigma$ there exists a sequence $(\kappa_{h,N})_{h,N} \subset \Lambda'$ of discrete eigenvalue to (3.15) converging to κ_0 .*
3. *For all $\kappa_0 \in \Lambda' \setminus \Sigma$ there exist constants $h_0, N_0, \varepsilon > 0$ such that the set $\{\kappa \in \Lambda' : |\kappa - \kappa_0| < \varepsilon\}$ contains no discrete eigenvalues for $h \leq h_0$ and $N \geq N_0$.*

Proof. Part 1: Let $(\kappa_{h,N}) \subset \Lambda$ be a sequence of discrete eigenvalues converging to $\kappa_0 \in \Lambda$ and assume that $\kappa_0 \notin \Sigma$. Then $\beta(\kappa_0) = \|T_{\kappa_0}^{-1}\|^{-1} > 0$, and by continuity of β at $\kappa = \kappa_0$ there exists $\varepsilon > 0$ such that $\inf\{\beta(\kappa) > 0 \mid \kappa \in \Lambda, |\kappa - \kappa_0| \leq \varepsilon\} > 0$. W.l.o.g. $B_\varepsilon(\kappa_0) := \{\kappa \in \mathbb{C} \mid |\kappa - \kappa_0| < \varepsilon\}$ is contained in some $\hat{\Lambda}$ from Assumption E. Then due to Lemma 4.4 there exist $h_0, N_0 > 0$ such that $\beta_{h,N}(\kappa_{h,N}) > 0$ for all $h \leq h_0$ and $N \geq N_0$. This implies that the unique solution to (3.15) for such h is $u_{h,N} = 0$, contradicting the assumption that $\kappa_{h,N}$ is a discrete eigenvalue.

Part 2: If $\kappa_0 \in \Sigma$, then $\beta(\kappa_0) = 0$ and due to discreteness of Σ and holomorphy of $\kappa \mapsto T_\kappa^{-1}$ on $\Lambda \setminus \Sigma$ there exists $\varepsilon > 0$ such that $\beta(\kappa) > 0$ for all $\kappa \in \overline{B_\varepsilon(\kappa_0)} \setminus \{\kappa_0\}$. Again, we may assume that the independence properties of Assumption E hold in $\overline{B_\varepsilon(\kappa_0)}$. By continuity of β and compactness of $\partial B_\varepsilon(\kappa_0)$ the number $\rho^\varepsilon := \min\{\beta(\kappa) \mid \kappa \in \partial B_\varepsilon(\kappa_0)\}$ is strictly positive. By Lemma 4.4 there exists $\rho > 0$ such that $\beta_{h,N}(\kappa) \geq \rho$ for all $\kappa \in \partial B_\varepsilon(\kappa_0)$, $h \leq h_0$ and $N \geq N_0$. Let $u_0 \in \mathcal{V}$ be an eigenvector corresponding to κ_0 , i.e. $s_{\kappa_0}(u_0, v) = 0$ for all $v \in \mathcal{V}$. Then with $C_\Lambda := \sup\{\|s_\kappa\| \mid \kappa \in \overline{\Lambda}\}$

$$\beta_{h,N}(\kappa_0) \leq \sup_{\substack{v \in \mathcal{V}_{h,N} \\ v \neq 0}} \frac{|s_{\kappa_0}(P_{h,N} u_0, v)|}{\|P_{h,N} u_0\|_{\mathcal{V}} \|v\|_{\mathcal{V}}} = \sup_{\substack{v \in \mathcal{V}_{h,N} \\ v \neq 0}} \frac{|s_{\kappa_0}(P_{h,N} u_0 - u_0, v)|}{\|P_{h,N} u_0\|_{\mathcal{V}} \|v\|_{\mathcal{V}}} \leq C_\Lambda \frac{\|P_{h,N} u_0 - u_0\|_{\mathcal{V}}}{\|P_{h,N} u_0\|_{\mathcal{V}}}.$$

The right hand side converges to 0, and hence for sufficiently small h and large N we have

$$\beta_{h,N}(\kappa) \geq \rho > \beta_{h,N}(\kappa_0) \quad \text{for all } \kappa \in \partial B_\varepsilon(\kappa_0). \quad (4.19)$$

Assume that for some such h there exist no discrete eigenvalues in $\overline{B_\varepsilon(\kappa_0)}$. Let \tilde{T}_κ be a matrix representing s on $\mathcal{V}_{h,N}$ with respect to some fixed basis. Then \tilde{T}_κ is invertible for all $\kappa \in B_\varepsilon(\kappa_0)$ and since \tilde{T}_κ depends holomorphically on κ , so does \tilde{T}_κ^{-1} .

Moreover, $\beta_{h,N}(\kappa) = \|\tilde{T}_\kappa^{-1}\|^{-1}$. It follows from Cauchy's integral formula $\tilde{T}_{\kappa_0}^{-1} = \frac{1}{2\pi i} \int_{\partial B_\varepsilon(\kappa_0)} \frac{d\kappa}{\kappa - \kappa_0} \tilde{T}_\kappa^{-1}$ that $\|\tilde{T}_{\kappa_0}^{-1}\| \leq \sup\{\|\tilde{T}_\kappa^{-1}\| : \kappa \in \partial B_\varepsilon(\kappa_0)\}$. This contradicts (4.19).

Part 3: Suppose the assertion is false for some $\kappa_0 \in \Lambda \setminus \Sigma$. Then there exists a sequence of discrete eigenvalues $(\kappa_{h,N})$ converging to κ_0 as $h \rightarrow 0$ and $N \rightarrow \infty$, and with the help of part 1 we obtain the contradiction $\kappa_0 \in \Sigma$. \square

With the help of Proposition 4.5 the proof of Theorem 3.4 is a straightforward compactness argument: Part 2 implies that $\sup_{\kappa \in \Sigma \cap \Lambda'} \inf_{\kappa_{h,N} \in \Sigma_{h,N} \cap \Lambda'} |\kappa - \kappa_{h,N}| \rightarrow 0$. Given $\delta > 0$ sufficiently small we can use compactness of Λ' to obtain a finite covering of $\Lambda' \setminus \bigcup_{\kappa \in \Sigma \cap \Lambda'} B_\delta(\kappa)$ by balls described in part 3. Since none of these balls contains a discrete eigenvalue in the limit $h \rightarrow 0$ and $N \rightarrow \infty$, it follows that $\sup_{\kappa_{h,N} \in \Sigma_{h,N} \cap \Lambda'} \inf_{\kappa \in \Sigma \cap \Lambda'} |\kappa - \kappa_{h,N}| \leq \delta$. As $\delta > 0$ was arbitrary, the limit is 0.

5 Complex scaling/ PML

In this section we first apply Theorem 3.2 to a Perfectly Matched Layer (PML) discretization of the diffraction problem (2.1) in Sec. 2. In the literature there exist already some convergence results for such problems (see e.g. [1]). However, in our approach the truncation error is treated as an approximation error and not as an error on the continuous level. Therefore, the techniques used in [1, 5, 13, 14, 16, 18] to handle this modeling error are not needed.

Moreover, since the PML method is better known than the Hardy space method presented in the next section, this section may help to follow the framework of the Hardy space method.

We will be particularly interested in complex frequencies $\kappa \in \mathbb{C}$ with positive real part representing the angular frequency and non positive imaginary part representing a damping in time. Since the radiation condition Def. 2.1 is only defined for positive frequencies κ , we have to define a proper holomorphic extension. Last we formulate the variational framework and prove the Assumptions A-E of Sec. 3. Theorem 3.2 and Theorem 3.4 yield convergence for discrete solutions to the diffraction problem as well as to the corresponding resonance problem.

5.1 complex scaling radiation condition

In this and the following subsection we consider for simplicity the case of a single waveguide $\Omega_{\text{ext}} := (0, \infty) \times \tilde{\Gamma}$ with left boundary $\Gamma := \{0\} \times \tilde{\Gamma}$, but without an interior domain:

$$-\Delta u^{\text{sc}} - \kappa^2 u^{\text{sc}} = 0 \quad \text{in } \Omega_{\text{ext}}, \quad (5.1a)$$

$$\mathcal{B} u^{\text{sc}} = 0 \quad \text{on } \partial\Omega_{\text{ext}} \setminus \Gamma, \quad (5.1b)$$

$$\frac{\partial u^{\text{sc}}}{\partial x} = g_{\text{in}} \quad \text{on } \Gamma, \quad (5.1c)$$

$$u^{\text{sc}} \text{ satisfies a radiation condition.} \quad (5.1d)$$

If we use the modal radiation condition (see Definition 2.1), then plugging (5.1c) into (2.3) yields $c_n = \langle g_{\text{in}}, \varphi_n \rangle_{L^2(\tilde{\Gamma})} / (i\kappa_n)$, and we obtain the unique solution

$$u^{\text{sc}}(x, y) = \sum_{n=1}^{\infty} \frac{\langle g_{\text{in}}, \varphi_n \rangle_{L^2(\tilde{\Gamma})}}{i\kappa_n} e^{i\kappa_n x} \varphi_n(y), \quad (x, y) \in \Omega_{\text{ext}}. \quad (5.2)$$

Definition 5.1 (complex scaling radiation condition). *Let $\sigma \in \mathbb{C}$ with $\Re(\sigma) > 0$ and $\Im(\sigma) > 0$ be the complex scaling parameter. A function $u \in H_{\text{loc}}^2(\Omega_{\text{ext}} \cup \Gamma)$ satisfies the complex scaling radiation condition with parameter σ if the mapping $(0, \infty) \rightarrow L^2(\tilde{\Gamma})$, $x \mapsto u(x, \cdot)$ has a holomorphic extension $\mathcal{S}_{\sigma} \rightarrow L^2(\tilde{\Gamma})$ to an open set $\mathcal{S}_{\sigma} \subset \mathbb{C}$ containing $\{z \in \mathbb{C} \setminus \{0\} \mid \arg(z) \in [0, \arg(\sigma)]\}$ and if the function*

$$u_{\sigma}(x, y) := u(\sigma x, y), \quad (x, y) \in \Omega_{\text{ext}}, \quad (5.3)$$

belongs to $H^2(\Omega_{\text{ext}})$.

Complex scaling was used in quantum physics since the 1970s (see e.g. [11, 20]) and reintroduced by Bérenger [2] under the name Perfectly Matched Layer (PML). For time-depending problems, the complex scaling parameter is typically chosen frequency dependent. Since for resonance problems this would lead to nonlinear eigenvalue problems, we avoid the incorporation of the frequency into the complex scaling. Moreover, due to the waveguide structure we may have several wavenumbers and it is not clear a priori, which of these should be used in the complex scaling.

Lemma 5.2. *Let $\sigma \in \mathbb{C}$ with $\Re(\sigma) > 0$ and $\Im(\sigma) > 0$ be any complex scaling parameter, let $\kappa > 0$, and assume (2.2). Then a solution $u^{\text{sc}} \in H_{\text{loc}}^1(\Omega_{\text{ext}} \cup \Gamma)$ to (5.1a), (5.1b), and (5.1c) satisfies the modal radiation condition (see Def. 2.1) if and only if it satisfies the complex scaling radiation condition with parameter σ (see Def. 5.1). In this case u_{σ} satisfies*

$$-\frac{1}{\sigma^2} \partial_x^2 u_{\sigma} - \Delta_{\tilde{\Gamma}} u_{\sigma} - \kappa^2 u_{\sigma} = 0 \quad \text{in } (0, \infty) \times \tilde{\Gamma}, \quad (5.4a)$$

$$\mathcal{B} u_{\sigma} = 0 \quad \text{on } (0, \infty) \times \partial \tilde{\Gamma}, \quad (5.4b)$$

$$\frac{\partial u_{\sigma}}{\partial x} = \sigma g_{\text{in}} \quad \text{on } \{0\} \times \tilde{\Gamma} \quad (5.4c)$$

and is given explicitly by

$$u_{\sigma}(x, y) = \sum_{n=1}^{\infty} \frac{\langle g_{\text{in}}, \varphi_n \rangle_{L^2(\tilde{\Gamma})}}{i\kappa_n} e^{i\sigma \kappa_n x} \varphi_n(y), \quad (x, y) \in \Omega_{\text{ext}}. \quad (5.5)$$

Vice versa, any solution $u_{\sigma} \in H^2(\Omega_{\text{ext}} \cup \Gamma)$ to (5.4) corresponds to the holomorphic extension of a solution to (5.1).

Proof. First assume that u^{sc} satisfies Def 2.1. To show that the right hand side of (5.2) is holomorphic in $x \in \mathbb{C} \setminus \{0\}$ if $\arg(x) \in [0, \arg(\sigma)]$ it suffices to show that the series and its formal complex derivative are absolutely convergent locally uniformly in x in the sense that for each x there exist $\varepsilon, C > 0$ such that $\sum_{n=1}^{\infty} |\langle g_{\text{in}}, \varphi_n \rangle|^2 \kappa_n^{-2} |e^{i\sigma \kappa_n \tilde{x}}|^2 \leq C$ and

$\sum_{n=1}^{\infty} |\langle g_{\text{in}}, \varphi_n \rangle|^2 |e^{i\sigma\kappa_n\tilde{x}}|^2 \leq C$ for all $\tilde{x} \in \mathbb{C}$ with $|x - \tilde{x}| < \varepsilon$. Note that $\Re(i\sigma\kappa_n) < 0$ for all $n \in \mathbb{N}$ and $\lim_{n \rightarrow \infty} \Re(i\sigma\kappa_n)/\sqrt{\lambda_n} = -\Re\sigma$. Hence the uniform bounds follow from the Weyl asymptotics of the eigenvalues λ_n and $\|g_{\text{in}}\|_{H^{1/2}} = \sum_{n=1}^{\infty} (1 + \lambda_n)^{1/2} |\langle g_{\text{in}}, \varphi_n \rangle|^2 < \infty$, i.e. the right hand side of (5.2) defines the required holomorphic extension. Moreover, it is easy to see that u_σ satisfies (5.4) and (5.5) and belongs to $H^2(\Omega_{\text{ext}})$.

Vice versa, assume that u^{sc} satisfies the complex scaling radiation condition. Since u^{sc} solves (5.1a) and (5.1b), the series representation (2.3) holds true. Since $x \mapsto u^{\text{sc}}(x, \cdot)$ has a $L^2(\tilde{\Gamma})$ -valued holomorphic extension, the mappings $x \mapsto \langle u^{\text{sc}}(x, \cdot), \varphi_n \rangle$ are also holomorphic. Therefore, they are given by $x \mapsto c_n \exp(i\kappa_n x) + d_n \exp(-i\kappa_n x)$, not only for $x \in (0, \infty)$, but also for $x \in \mathcal{S}_\sigma$, i.e. the holomorphic extension of u^{sc} is given by the right hand side of (2.3) with $x \in \mathcal{S}_\sigma$. As

$$u_\sigma(x, y) = \sum_{n=1}^{\infty} (c_n e^{i\sigma\kappa_n x} + d_n e^{-i\sigma\kappa_n x}) \varphi_n(y) \quad \text{in } \Omega_{\text{ext}},$$

the assumption $u_\sigma \in H^2(\Omega_{\text{ext}})$ implies $d_n = 0$ for all $n \in \mathbb{N}$, i.e. u^{sc} satisfies the modal radiation condition.

Given a solution $u_\sigma \in H^2(\Omega_{\text{ext}} \cup \Gamma)$ to (5.4) we can conclude that it is of the form (5.5), and hence corresponds to a holomorphic extension of a solution to (5.1). \square

Note that the holomorphic extension in Def. 5.1 does not appear explicitly in numerical computations since such computations are based on (5.4).

5.2 complex scaling radiation condition for complex frequencies

For complex frequencies κ the choice of the branch cut of the square root function is not canonical, and different choices may lead to different modal radiation conditions. Similarly, different choices of σ may lead to different complex scaling radiation conditions: A solution $u_\sigma \in H^2(\Omega_{\text{ext}})$ to (5.4) with complex κ is given by (5.5), if $\kappa_n = \sqrt{\kappa^2 - \lambda_n}$ is defined such that $\Re(i\sigma\kappa_n) < 0$. Hence, we are led to the following definition.

Definition 5.3. For $\sigma = |\sigma| \exp(i \arg(\sigma)) \in \mathbb{C}$ with $\arg : \mathbb{C} \rightarrow [-\pi, \pi)$ and $\arg(\sigma) \in (0, \frac{\pi}{2})$ we define

$$\sqrt{z}^\sigma := \sqrt{|z|} e^{i\frac{\varphi}{2}} \quad \text{for } z = |z| e^{i\varphi} \text{ with } \varphi \in [-2\arg(\sigma), 2\pi - 2\arg(\sigma)). \quad (5.6)$$

If $\lambda_1 \leq \lambda_2 \leq \dots$ denote the eigenvalues of $-\Delta_\Gamma$, we define $\kappa_n^\sigma : \mathbb{C} \rightarrow \mathbb{C}$ for $n \in \mathbb{N}$ by $\kappa_n^\sigma = \kappa_n^\sigma(\kappa) := \sqrt{\kappa^2 - \lambda_n}^\sigma$.

By definition we have $\Re(i\sigma\kappa_n^\sigma) \leq 0$ for all $n \in \mathbb{N}$. We can define similar to Def 2.1 a complex modal radiation condition: A function u of the form

$$u(x, y) = \sum_{n=1}^{\infty} (c_n e^{i\kappa_n^\sigma x} + d_n e^{-i\kappa_n^\sigma x}) \varphi_n(y), \quad (x, y) \in \Omega_{\text{ext}}, \quad (5.7)$$

satisfies the modal radiation condition if all coefficients d_n vanish. As in Lemma 5.2 equivalence of this modal radiation condition to the complex scaling radiation condition Def. 5.1 can be shown if $\Re(i\sigma\kappa_n^\sigma) \neq 0$ for all $n \in \mathbb{N}$.

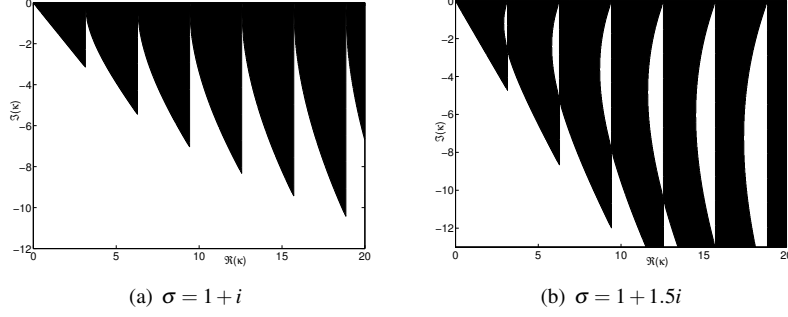


Figure 2: admissible sets $\Lambda_{\Delta_\Gamma}^\sigma$ for two different σ and $\lambda_n = (n-1)^2\pi^2$, $n \in \mathbb{N}$

Nevertheless, if we would use this definition without any restrictions, we would get different solutions u^{sc} (see (5.2)) to (5.1) for different PML parameters σ . In other words, different σ yield different radiation conditions. To avoid this undesirable effect, we define admissible regions for κ , such that $\kappa_n^{\sigma_1} = \kappa_n^{\sigma_2}$ for $\sigma_1, \sigma_2 \in \mathbb{C}$.

Definition 5.4. Let $\lambda_1 \leq \lambda_2 \leq \dots$ denote the eigenvalues of $-\Delta_\Gamma$ and κ_n^σ as defined in Def.5.3. The admissible set $\Lambda_{\Delta_\Gamma}^\sigma \subset \mathbb{C}$ is the set of all $\kappa \in \mathbb{C}$ with $\Re \kappa > 0$ and $\Im \kappa \leq 0$ such that

1. κ_n^σ is holomorphic at κ and
2. κ_n^σ is continuous along the path $\{\Re(\kappa) - ti \in \mathbb{C} \mid t \in (0, -\Im(\kappa))\}$.

for all $n \in \mathbb{N}$.

For $\kappa \in \Lambda_{\Delta_\Gamma}^{\sigma_1} \cap \Lambda_{\Delta_\Gamma}^{\sigma_2}$ the modal radiation conditions with parameters σ_1 and σ_2 coincide, since for all $n \in \mathbb{N}$ $\sqrt{\Re(\kappa)^2 - \lambda_n}^{\sigma_1} = \sqrt{\Re(\kappa)^2 - \lambda_n}^{\sigma_2}$ and none of the paths $\{(\Re(\kappa) - ti)^2 - \lambda_n \in \mathbb{C} \mid t \in (0, -\Im(\kappa))\}$ has passed the branch cuts of $\sqrt{\cdot}^{\sigma_1}$ and $\sqrt{\cdot}^{\sigma_2}$.

In Fig. 2 two admissible sets are given for a two-dimensional waveguide $\mathbb{R}_+ \times [0, 1]$. For $\sigma = 1 + i$ the branch cut of the square root is the negative imaginary axis, and therefore only in absolute values small imaginary parts of κ are allowed if $\Re(\kappa)$ is a little bit larger than on $\sqrt{\lambda_n}$ (see Fig. 2(a)). For $\sigma = 1 + 1.5i$ the branch cut of the square root is in the third quadrant and therefore κ with $\Re(\kappa)$ a little bit smaller than one $\sqrt{\lambda_n}$ are more problematic (see Fig. 2(b)).

Note, that $\Lambda_{\Delta_\Gamma}^\sigma$ is the union of the disjoint sets

$$(\Lambda_{\Delta_\Gamma}^\sigma)^n := \left\{ \kappa \in \mathbb{C} \mid \Re(\kappa) > 0, \Im(\kappa) \leq 0, \sqrt{\lambda_n} < \Re(\kappa) < \sqrt{\lambda_{n+1}}, \right. \\ \left. \arg(\kappa^2 - \lambda_{n+1}) < -2\arg(\sigma) < \arg(\kappa^2 - \lambda_n) \right\}. \quad (5.8)$$

5.3 convergence of the PML method

In the case of several waveguides $W_l = \eta_l((0, \infty) \times \tilde{\Gamma}_l)$ for $l = 1, \dots, L$ (see Sec. 2), we use the complex scaling vector $\sigma = (\sigma_1, \dots, \sigma_L) \in \mathbb{C}^L$ with $\Re(\sigma_l), \Im(\sigma_l) > 0$ and define for a solution u to (2.1) $u^{\text{int}} := u|_{\Omega_{\text{int}}}$,

$$u_l^{(\sigma_l)}(x, y) := u|_{W_l} \circ \eta_l(\sigma_l x, y), \quad (x, y) \in (0, \infty) \times \tilde{\Gamma}_l, \quad l = 1, \dots, L,$$

and $u_\sigma^{\text{ext}} := (u_1^{(\sigma_1)}, \dots, u_L^{(\sigma_L)})^\top$. The admissible set will be

$$\Lambda := \bigcap_{l=1}^L \Lambda_{\Delta_l}^{\sigma_l}. \quad (5.9)$$

Let us formally state our definition of resonances:

Definition 5.5. $\kappa \in \Lambda$ (for some scaling parameters σ_l) is called a resonance if there exists a resonance function $u \in H_{\text{loc}}^1(\Omega) \setminus \{0\}$ satisfying $-\Delta u = \kappa^2 u$ in Ω , $\mathcal{B}u = 0$ on $\partial\Omega$ and the complex scaling radiation condition with parameter σ_l in each waveguide W_l .

We will check point by point the assumptions of Sec. 3 for a complex scaled version of (2.1). For notational simplicity we again discuss only the case of Dirichlet boundary conditions, i.e. $\mathcal{B}u := u|_{\partial\Omega}$.

Assumption A: Exterior and interior spaces. $\mathcal{V}^{\text{int}, \text{tr}_-}$ and \mathcal{Z} are defined as in Section 3 after Ass. A with $\Gamma = \bigcup_{l=1}^L \Gamma_l$. We define $\mathcal{V}^{\text{ext}} = \bigoplus_{l=1}^L \mathcal{V}_l^{\text{ext}}$ with

$$\mathcal{V}_l^{\text{ext}} := \{u_l^{\text{ext}} \in H^1((0, \infty) \times \tilde{\Gamma}_l) : u_l^{\text{ext}}|_{(0, \infty) \times \partial\tilde{\Gamma}_l} = 0\}.$$

The spaces $\mathcal{X}_l^1, \mathcal{X}_l^2, \mathcal{Y}_l^1$ and \mathcal{Y}_l^2 are defined as in Sec. 3. The trace operator $\text{tr}_+ : \mathcal{V}^{\text{ext}} \rightarrow \mathcal{Z}$ is defined for $u^{\text{ext}} = (u_1^{\text{ext}}, \dots, u_L^{\text{ext}})^\top \in \mathcal{V}^{\text{ext}}$ point wise: For $y \in \Gamma$ we choose $l \in \{1, \dots, L\}$ such that $y = \eta_l(0, \tilde{y}) \in \Gamma_l$ with $\tilde{y} \in \tilde{\Gamma}_l$ and define $(\text{tr}_+ u^{\text{ext}})(y) := u_l^{\text{ext}}(0, \tilde{y})$.

Finally, we define the bounded sesquilinear forms

$$\begin{aligned} a^{\text{int}}(u^{\text{int}}, v^{\text{int}}) &:= \int_{\Omega_{\text{int}}} \nabla u^{\text{int}} \cdot \nabla \overline{v^{\text{int}}} dx, & b^{\text{int}}(u^{\text{int}}, v^{\text{int}}) &:= \int_{\Omega_{\text{int}}} u^{\text{int}} \overline{v^{\text{int}}} dx \\ a_l^{\text{ext}}(u_l^{\text{ext}}, v_l^{\text{ext}}) &:= \int_0^\infty \int_{\tilde{\Gamma}_l} \left(\frac{1}{\sigma_l} \partial_x u_l^{\text{ext}} \partial_x \overline{v_l^{\text{ext}}} + \sigma_l \nabla_y u_l^{\text{ext}} \cdot \nabla_y \overline{v_l^{\text{ext}}} \right) dy dx, \\ b_l^{\text{ext}}(u_l^{\text{ext}}, v_l^{\text{ext}}) &:= \int_0^\infty \int_{\tilde{\Gamma}_l} \sigma_l u_l^{\text{ext}} \overline{v_l^{\text{ext}}} dy dx, \end{aligned}$$

and set $s^{\text{int}} := a^{\text{int}} - \kappa^2 b^{\text{int}}, s_l^{\text{ext}} := a_l^{\text{ext}} - \kappa^2 b_l^{\text{ext}}$ and $s^{\text{ext}}(u^{\text{ext}}, v^{\text{ext}}) := \sum_{l=1}^L s_l^{\text{ext}}(u_l^{\text{ext}}, v_l^{\text{ext}})$ for $u^{\text{ext}} = (u_1^{\text{ext}}, \dots, u_L^{\text{ext}})^\top$ and $v^{\text{ext}} = (v_1^{\text{ext}}, \dots, v_L^{\text{ext}})^\top$.

Using these definitions we arrive at the PML variational formulation: If $\kappa \in \Lambda$ then u is a solution to (2.1) with the complex scaling radiation condition with parameter σ_l in each waveguide W_l if and only if $(u^{\text{int}}, u_\sigma^{\text{ext}})^\top \in \mathcal{V}$ solves

$$s \left(\begin{pmatrix} u^{\text{int}} \\ u_\sigma^{\text{ext}} \end{pmatrix}, \begin{pmatrix} v^{\text{int}} \\ v_\sigma^{\text{ext}} \end{pmatrix} \right) = F \left(\begin{pmatrix} v^{\text{int}} \\ v_\sigma^{\text{ext}} \end{pmatrix} \right), \quad \begin{pmatrix} v^{\text{int}} \\ v_\sigma^{\text{ext}} \end{pmatrix} \in \mathcal{V}, \quad (5.10)$$

with

$$F\left(\left(\begin{smallmatrix} \text{int} \\ v^{\text{ext}} \end{smallmatrix}\right)\right) := \int_{\Omega_{\text{int}}} f \overline{v^{\text{int}}} dx + \sum_{l=1}^L \int_{\Gamma_l} \frac{\partial u^{\text{inc}}}{\partial \nu} \overline{v^{\text{int}}} ds + \sum_{l=1}^L s_l^{\text{ext}} \left(\left(E_{+,l} u^{\text{inc}}|_{\Gamma_l} \right) \circ \eta_l, v_l^{\text{ext}} \right).$$

$E_{+,l} : \mathcal{X}_l \rightarrow \mathcal{V}_l^{\text{ext}}$ can be any bounded extension operator with bounded support $\{x \in W_l \mid (E_{+,l}f)(x) \neq 0, f \in \mathcal{X}_l\}$ in W_l .

Moreover, with the help of the generalization of Lemma 5.2 to complex κ we can show that $\kappa \in \Lambda$ is a resonance if and only if there exists $u \in \mathcal{V} \setminus \{0\}$ such that

$$s_\kappa(u, v) = 0 \quad \text{for all } v \in \mathcal{V}.$$

Assumption B: separation of \mathcal{V}^{ext} . In order to simplify the presentation, we only consider the case of one waveguide $W_1 = (0, \infty) \times \tilde{\Gamma}$ in the following and omit the lower index 1 for $l = 1$. As in Sec. 3 we use the orthogonal set of eigenfunctions $\{\varphi_n : n \in \mathbb{N}\} \subset \mathcal{D}^2$ to $-\Delta$, i.e. $-\Delta \varphi_n = \lambda_n \varphi_n$ with $\lambda_n \geq 0$. The orthogonality assumptions are trivial. The norms of \mathcal{X}_n and the separated sesquilinear forms are given by

$$\|u\|_{\mathcal{X}_n}^2 = \|u'\|_{L^2}^2 + (\lambda_n + 2)\|u\|_{L^2}^2, \quad s_n(u, v) = \frac{1}{\sigma} \langle u', v' \rangle_{L^2} + \sigma(\lambda_n - \kappa^2) \langle u, v \rangle_{L^2}. \quad (5.11)$$

Assumption C: boundedness and coercivity. s_n is bounded by

$$|s_n(u, v)| \leq \max\left(\frac{1}{|\sigma|} + |\sigma \kappa^2|, |\sigma|\right) \|u\|_{\mathcal{X}_n} \|v\|_{\mathcal{X}_n} \quad (5.12)$$

with a constant independent of n . For the coercivity we consider each of the disjoints sets of $\Lambda_{\Delta\Gamma}^\sigma$ defined in (5.8) separately: For $n_0 \in \mathbb{N}$ and $\kappa \in \left(\Lambda_{\Delta\Gamma}^\sigma\right)^{n_0}$ it holds

$$-\pi \leq \arg(\kappa^2 - \lambda_{n_0+1}) < -2\arg(\sigma) < \arg(\kappa^2 - \lambda_{n_0}) \leq 0. \quad (5.13)$$

Note, that $n \mapsto \arg(\kappa^2 - \lambda_n) \in [-\pi, 0]$ is monotonically decreasing since $\lambda_n \rightarrow \infty$ for $n \rightarrow \infty$. We distinguish two cases which for $\kappa > 0$ correspond exactly to the cases of propagating modes ($\kappa^2 > \lambda_n$) and evanescent modes ($\kappa^2 < \lambda_n$): $n \leq n_0$ and $n > n_0$.

1. For $n = 1, \dots, n_0$ the right half of (5.13) leads to

$$-\arg(\sigma) < \arg(\kappa^2 - \lambda_n) + \arg(\sigma) = \arg(\sigma(\kappa^2 - \lambda_n)) \leq \arg(\sigma), \quad (5.14)$$

since $\arg(\sigma) \in (0, \frac{\pi}{2})$ and $\arg(\kappa^2 - \lambda_n) \in (-\pi, 0]$. We define the rotations of (3.7b) by

$$\theta_n(\kappa) := \exp\left(i \left(\frac{\pi + \arg(\sigma) - \arg(\sigma(\kappa^2 - \lambda_n))}{2} \right)\right)$$

and compute

$$\begin{aligned} \frac{\theta_n}{\sigma} &= \frac{1}{|\sigma|} \exp\left(i \left(\frac{\pi - \arg(\sigma) - \arg(\sigma(\kappa^2 - \lambda_n))}{2} \right)\right), \\ -\theta_n \sigma(\kappa^2 - \lambda_n) &= -\exp\left(i \left(\frac{\pi + \arg(\sigma) + \arg(\sigma(\kappa^2 - \lambda_n))}{2} \right)\right). \end{aligned}$$

Using (5.14) we get

$$\alpha_n(\kappa) := \min \left\{ \Re \left(\frac{\theta_n(\kappa)}{\sigma} \right), \frac{\Re(\theta_n(\kappa)\sigma(\lambda_n - \kappa^2))}{2 + \lambda_n} \right\} > 0$$

and (3.7b) is shown for the separated sesquilinear forms s_n defined in (5.11).

2. For $n = n_0 + 1, \dots$ we take the left half of (5.13), use $0 > \arg(\sigma(\kappa^2 - \lambda_n)) = \arg(\sigma(\lambda_n - \kappa^2)) - \pi$ and deduce

$$\arg(\sigma) \leq \arg(\sigma(\lambda_n - \kappa^2)) < \pi - \arg(\sigma). \quad (5.15)$$

Since $(\Lambda_{\Delta_\Gamma}^\sigma)^{n_0}$ is bounded (see Fig. 2) and $\lambda_j \rightarrow \infty$ for $j \rightarrow \infty$ there exists a constant $M^{n_0} \in \mathbb{N}$ defined by

$$M^{n_0} := \min \left\{ j \in \mathbb{N} \mid \lambda_{j+1} > 2 \frac{\Re(\sigma \kappa^2)}{\Re(\sigma)} \text{ for all } \kappa \in (\Lambda_{\Delta_\Gamma}^\sigma)^{n_0} \right\}.$$

For $n > M^{n_0}$ there holds $\Re(\sigma(\lambda_n - \kappa^2)) > \frac{\Re(\sigma)}{2} \lambda_n$ and (3.7c) holds true with

$$\alpha_n := \min \left\{ \frac{1}{\Re(\sigma)}, \frac{\Re(\sigma) \lambda_n}{4 + 2 \lambda_n} \right\} > 0.$$

For $n = n_0 + 1, \dots, M^{n_0}$ we define similar to the first case

$$\theta_n(\kappa) := \exp \left(i \left(\frac{\arg(\sigma) - \arg(\sigma(\lambda_n - \kappa^2))}{2} \right) \right)$$

and use (5.15) for

$$\alpha_n(\kappa) := \min \left\{ \Re \left(\frac{\theta_n(\kappa)}{\sigma} \right), \frac{\Re(\theta_n(\kappa)\sigma(\lambda_n - \kappa^2))}{2 + \lambda_n} \right\} > 0.$$

Since $\alpha_n \rightarrow \min \left\{ \frac{1}{\Re(\sigma)}, \frac{\Re(\sigma)}{2} \right\}$ for $n \rightarrow \infty$, the constant $\alpha(\kappa) := \inf \{ \alpha_n(\kappa) \mid n \in \mathbb{N} \}$ in (3.7b) and (3.7c) is strictly positive.

Assumption D: discrete subspaces. The discrete subspaces are chosen exactly the same way as in Section 3.

Assumption E: eigenvalue setting. Most properties stated in this assumption are obvious, but we have to argue that C_s, θ_n, α and M can be chosen independent of κ in a neighborhood $\widehat{\Lambda}$ of each $\kappa_0 \in \Lambda$. If $\widehat{\Lambda} \subset (\Lambda_{\Delta_\Gamma}^\sigma)^n$ for one $n \in \mathbb{N}$, then M is independent of $\kappa \in \widehat{\Lambda}$. Due to (5.14) and (5.15) θ_n depends continuously on κ . The same holds true for C_s and α . Therefore, they can be chosen independent of $\kappa \in \widehat{\Lambda}$ if $\widehat{\Lambda}$ is compact.

Since all assumptions are satisfied, Theorem 3.2 is applicable and yields the following:

Theorem 5.6 (PML for diffraction problems). *If $\kappa \in \Lambda$ with Λ defined in (5.9) is not a resonance, then equation (5.10) is uniquely solvable with solution $(u^{\text{int}}, u^{\text{ext}})^\top \in \mathcal{V}$ for all right hand sides $F \in \mathcal{V}^*$, and there exists a constant $h_0 > 0$ such that the discrete variational problems*

$$a\left(\begin{pmatrix} u_h^{\text{int}} \\ u_{h,N}^{\text{ext}} \end{pmatrix}, \begin{pmatrix} v_h^{\text{int}} \\ v_{h,N}^{\text{ext}} \end{pmatrix}\right) - \kappa^2 b\left(\begin{pmatrix} u_h^{\text{int}} \\ u_{h,N}^{\text{ext}} \end{pmatrix}, \begin{pmatrix} v_h^{\text{int}} \\ v_{h,N}^{\text{ext}} \end{pmatrix}\right) = F\left(\begin{pmatrix} v_h^{\text{int}} \\ v_{h,N}^{\text{ext}} \end{pmatrix}\right), \quad \begin{pmatrix} v_h^{\text{int}} \\ v_{h,N}^{\text{ext}} \end{pmatrix} \in \mathcal{V}_{h,N} \quad (5.16)$$

have a unique solution $(u_h^{\text{int}}, u_{h,N}^{\text{ext}})^\top \in \mathcal{V}_{h,N}$ for all $h \leq h_0$ and all $N \in \mathbb{N}$. Moreover, there exists a constant $C > 0$ independent of h and N such that

$$\left\| \begin{pmatrix} u^{\text{int}} \\ u^{\text{ext}} \end{pmatrix} - \begin{pmatrix} u_h^{\text{int}} \\ u_{h,N}^{\text{ext}} \end{pmatrix} \right\|_{\mathcal{V}} \leq C \inf_{(w_h^{\text{int}}, w_{h,N}^{\text{ext}})^\top \in \mathcal{V}_{h,N}} \left\| \begin{pmatrix} u^{\text{int}} \\ u^{\text{ext}} \end{pmatrix} - \begin{pmatrix} w_h^{\text{int}} \\ w_{h,N}^{\text{ext}} \end{pmatrix} \right\|_{\mathcal{V}}.$$

Part of the approximation error is the error due to truncation of the infinite PML. In each waveguide W_l , $l = 1, \dots, L$, we approximate (cf. (5.5))

$$\tilde{u}_l(x, y) := \sum_{n=1}^{\infty} c_n e^{i\sigma_l \sqrt{\kappa^2 - \lambda_n^l} x} \phi_n^l(y), \quad (x, y) \in (0, \infty) \times \tilde{\Gamma}_l,$$

by 0 for all $x \geq \rho_N, y \in \tilde{\Gamma}_l$ (ρ_N being the length of the PML defined in Sec. 3 after Ass. D). Hence, suppressing the indices l the truncation error can be estimated by

$$\|\tilde{u}\|_{H^1((\rho, \infty) \times \tilde{\Gamma})}^2 \leq \sum_{n=1}^{\infty} |c_n|^2 \left(|\kappa_n^\sigma \sigma|^2 + \frac{1 + \lambda_n}{-2\Re(i\kappa_n^\sigma \sigma)} \right) e^{2\Re(i\kappa_n^\sigma \sigma) \rho_N} \quad (5.17)$$

with κ_n^σ defined in Def. 5.3. Due to $\Re(i\kappa_n^\sigma \sigma) < 0$ the truncation error is exponentially decreasing with increasing ρ_N . Nevertheless, the error becomes large, if $\Re(i\sqrt{\kappa^2 - \lambda_n} \sigma) \approx 0$ for some n , which is the case for $\kappa^2 \approx \lambda_n$ as well as near the branch cuts of the square root.

Theorem 3.4 yields the following:

Theorem 5.7 (PML for resonance problems). *For all compact $\Lambda' \subset \Lambda$ we have*

$$\lim_{h \rightarrow 0, N \rightarrow \infty} \text{dist}(\Sigma \cap \Lambda', \Sigma_{h,N} \cap \Lambda') = 0.$$

Proof. What remains to be shown is that there exists a κ such that (5.10) is uniquely solvable. s_κ depends holomorphically on κ for $\kappa \in \Lambda \cup \{z \in \mathbb{C} : \arg(z) \in (0, \frac{\pi}{2})\}$. Since Ass. C can be shown for $\kappa \in \{z \in \mathbb{C} : \arg(z) \in (0, \frac{\pi}{2})\}$ similar to $\kappa \in \Lambda$, we can use Theorem 3.4 for $\Lambda \cup \{z \in \mathbb{C} : \arg(z) \in (0, \frac{\pi}{2})\}$. Since for κ with $0 < \Re(\kappa) < \Im(\kappa)$ the real parts of all the coefficients in s_κ are positive, i.e.

$$\min \left\{ 1, \Re(-\kappa^2), \Re\left(\frac{1}{\sigma}\right), \min_{n \in \mathbb{N}} \Re\left(\frac{\sigma(\lambda_n - \kappa^2)}{2 + \lambda_n}\right) \right\} > 0,$$

(5.10) is for such κ uniquely solvable by the Lax-Milgram Lemma and the proof is complete. \square

6 Hardy space method

As in the previous section we first introduce another equivalent formulation of the radiation condition called the pole condition. Based on the pole condition we formulate the Hardy space variational problem and use Theorem 3.2 to show an exponential convergence with respect to the number of degrees of freedom in radial direction. We end this section with the description of a suitable choice of the approximating subspace which avoids deterioration of convergence for frequencies close to Wood anomalies.

6.1 pole condition

For the discussion of the pole condition we again consider only one waveguide as in §5.1. Let $u^{\text{sc}}(x, y) = \sum_{n=1}^{\infty} c_n e^{i\kappa_n x} \varphi_n(y)$ be a solution to (5.1a) and (5.1b) with $\kappa > 0$ satisfying the modal radiation condition. Then the Laplace transform $\hat{u}(s, y) := \mathcal{L}(u^{\text{sc}}(\cdot, y))(s)$ of u^{sc} in the infinite direction x is given by

$$\hat{u}(s, y) = \sum_{n=1}^{\infty} \frac{c_n}{s - i\kappa_n} \varphi_n(y), \quad \Re(s) > 0, \quad y \in \tilde{\Gamma}.$$

It has a meromorphic extension to \mathbb{C} with poles at $\{i\kappa_n, n \in \mathbb{N}\}$. In contrast, the Laplace transform of $e^{-i\kappa_n x}$ has a pole at $-i\kappa_n$. Since for real κ the numbers $i\kappa_n$ lie on the positive imaginary axis and the negative real axis, formally u^{sc} satisfies the modal radiation condition if and only if \hat{u} has no poles in a complex half plane $\{\kappa_0 s : s \in \mathbb{C}, \Im s < 0\}$ for some $\kappa_0 \in \mathbb{C}$ with $\Re \kappa_0 > 0, \Im \kappa_0 > 0$, which will be a parameter of the method.

We define the Möbius mapping $m_{\kappa_0} : \mathbb{C} \setminus \{1\} \rightarrow \mathbb{C}$, $m_{\kappa_0}(z) := i\kappa_0 \frac{z+1}{z-1}$ and a corresponding Möbius transform $\mathcal{M}_{\kappa_0} : L^2(\kappa_0 \mathbb{R}) \rightarrow L^2(S^1)$ from $\kappa_0 \mathbb{R} := \{\kappa_0 s \mid s \in \mathbb{R}\}$ to the complex unit sphere $S^1 := \{z \in \mathbb{C} \mid |z| = 1\}$ via

$$(\mathcal{M}_{\kappa_0} f)(z) := \frac{(f \circ m_{\kappa_0})(z)}{z - 1}, \quad z \in S^1 \setminus \{1\}, \quad f \in L^2(\kappa_0 \mathbb{R}).$$

Due to the scaling $(z - 1)^{-1}$ the Möbius transform \mathcal{M}_{κ_0} is unitary up to a constant. Applying \mathcal{M}_{κ_0} to the Laplace transformed function \hat{u} we get

$$(\mathcal{M}_{\kappa_0} \hat{u})(z) = \sum_{n=1}^{\infty} \frac{c_n \varphi_n(y)}{i(\kappa_0 - \kappa_n)z + i(\kappa_n + \kappa_0)}, \quad z \in S^1, \quad y \in \tilde{\Gamma}. \quad (6.1)$$

The Hardy space $H^+(S^1)$ is defined as the set of all functions $f \in L^2(S^1)$ for which there exists a holomorphic function $v : \{z \in \mathbb{C} \mid |z| < 1\} \rightarrow \mathbb{C}$ such that $\lim_{r \nearrow 1} \int_0^{2\pi} |v(re^{it}) - f(e^{it})|^2 dt = 0$. Equipped with the L^2 -inner product, $H^+(S^1)$ is a Hilbert space (see e.g. [6]).

Definition 6.1 (pole condition). *Let $\kappa_0 \in \mathbb{C}$ with $\Re \kappa_0 > 0$ and $\Im \kappa_0 > 0$. A function $u \in H_{\text{loc}}^2(\Omega_{\text{ext}} \cup \Gamma)$ satisfies the pole condition with parameter κ_0 if*

$$\int_0^\infty e^{-s_0 x} \|u(x, \cdot)\|_{L^2(\tilde{\Gamma})} dx < \infty$$

for some $s_0 > 0$ and the Laplace transform $(\mathcal{L}u)(s) := \int_0^\infty e^{-sx} u(x, \cdot) dx$ (with values in $L^2(\tilde{\Gamma})$) has a holomorphic extension from $\{s \in \mathbb{C} : \Re s > s_0\}$ to the half-plane $\{\kappa_0 s : s \in \mathbb{C}, \Im s < 0\}$ with L^2 -boundary values on $\kappa_0 \mathbb{R}$ such that

$$\mathcal{M}_{\kappa_0} \mathcal{L}u \in H^+(S^1) \otimes L^2(\tilde{\Gamma}).$$

Lemma 6.2. *Let $\kappa \in \mathbb{C}$ with $\Re(\kappa) > 0$ and $\Im(\kappa) \leq 0$ and let $u^{\text{sc}} \in H_{\text{loc}}^1(\Omega_{\text{ext}} \cup \Gamma)$ be a solution to (5.1a) and (5.1b) with expansion (5.7) using the definition of κ_n^σ of Definition 5.3 with $\sigma := i/\kappa_0$. Moreover, let κ belong to the admissible set $\Lambda_{\Delta_\Gamma}^\sigma$ defined in Def. 5.4. Then the following statements are equivalent:*

1. (modal radiation condition) All coefficients d_n in (5.7) vanish.
2. u^{sc} satisfies the pole condition with parameter κ_0 .

Proof. By definition of κ_n^σ and $\kappa \in \Lambda_{\Delta_\Gamma}^\sigma$ there holds

$$\Re(\kappa_n^\sigma / \kappa_0) > 0 \quad \text{and} \quad \left| \frac{\kappa_n^\sigma + \kappa_0}{\kappa_n^\sigma - \kappa_0} \right| > 1 \quad \text{for all } n \in \mathbb{N}. \quad (6.2)$$

First assume that u^{sc} satisfies the modal radiation condition. Then $\mathcal{M}_{\kappa_0} \mathcal{L}u^{\text{sc}}$ is well defined and satisfies (6.1) with $\kappa_n = \kappa_n^\sigma$. Therefore, each term in the series (6.1) belongs to $H^+(S^1) \otimes L^2(\tilde{\Gamma})$. Moreover, the series converges in $L^2(S^1) \otimes L^2(\tilde{\Gamma})$ since $\left\| \frac{1}{i(\kappa_0 - \kappa_n^\sigma)z + i(\kappa_n^\sigma + \kappa_0)} \right\|_{L^2(S^1)} = \mathcal{O}\left(\frac{1}{|\kappa_n^\sigma|}\right) = \mathcal{O}\left(\lambda_n^{-1/2}\right)$ (see [12, proof of Lemma A.3]) and $\sum_{n=1}^\infty (1 + \lambda_n)^{1/2} |c_n|^2 = \|u|_\Gamma\|_{H^{1/2}(\Gamma)}^2 < \infty$.

Vice versa assume that u^{sc} satisfies the pole condition. Then

$$\frac{c_n}{i(\kappa_0 - \kappa_n^\sigma)z + i(\kappa_n^\sigma + \kappa_0)} + \frac{d_n}{i(\kappa_0 + \kappa_n^\sigma)z - i(\kappa_n^\sigma - \kappa_0)} = \mathcal{M}_{\kappa_0} \mathcal{L} \langle u^{\text{sc}}, \varphi_n \rangle_{L^2(\tilde{\Gamma})} \in H^+(S^1)$$

for all $n \in \mathbb{N}$. Since $z \mapsto (i(\kappa_0 + \kappa_n^\sigma)z - i(\kappa_n^\sigma - \kappa_0))^{-1}$ has a pole at $\frac{\kappa_n^\sigma - \kappa_0}{\kappa_n^\sigma + \kappa_0} \in \{z \in \mathbb{C} : |z| < 1\}$, it follows that $d_n = 0$. \square

Note that $s_0 > 0$ in Def. 6.1 is needed for frequencies κ with $\Im \kappa < 0$ since by definition of κ_n^σ propagating modes become exponentially increasing in this case. However, the pole condition is independent of the choice of s_0 .

6.2 Hardy space variational formulation for one waveguide

For the details of the Hardy space method in one dimension we refer to [12, sec. 2]. The role of the damping parameter σ is replaced in the HSM by the parameter $\kappa_0 \in \mathbb{C}$ of the Möbius transform, which satisfies $\Re(\kappa_0) > 0$ and $\Im(\kappa_0) > 0$.

For simplicity we introduce the linear, injective and bounded operators $\mathcal{T}_\pm : \mathbb{C} \oplus H^+(S^1) \rightarrow H^+(S^1)$ by

$$(\mathcal{T}_\pm \begin{pmatrix} f_0 \\ F \end{pmatrix})(z) := \frac{1}{2}(f_0 + (z \pm 1)F(z)), \quad z \in S^1, \quad \begin{pmatrix} f_0 \\ F \end{pmatrix} \in \mathbb{C} \oplus H^+(S^1) \quad (6.3)$$

and recall the equations (2.9) and (2.14) from [12, sec. 2]: For suitable $f : [0, \infty) \rightarrow \mathbb{C}$ and $f_0 := f(0)$ there exists a $F \in H^+(S^1)$ such that

$$\mathcal{M}_{\kappa_0} \mathcal{L} f = \frac{1}{i\kappa_0} \mathcal{T}_- \begin{pmatrix} f_0 \\ F \end{pmatrix} \quad \text{and} \quad \mathcal{M}_{\kappa_0} \mathcal{L} \partial_x f = \mathcal{T}_+ \begin{pmatrix} f_0 \\ F \end{pmatrix}. \quad (6.4)$$

Due to the boundedness of \mathcal{T}_\pm and the parallelogram identity, there exist constants $C_1, C_2 > 0$ such that

$$C_1 \left\| \begin{pmatrix} f_0 \\ F \end{pmatrix} \right\|_{\mathbb{C} \oplus L^2(S^1)}^2 \leq \left\| \mathcal{T}_+ \begin{pmatrix} f_0 \\ F \end{pmatrix} \right\|_{L^2(S^1)}^2 + \left\| \mathcal{T}_- \begin{pmatrix} f_0 \\ F \end{pmatrix} \right\|_{L^2(S^1)}^2 \leq C_2 \left\| \begin{pmatrix} f_0 \\ F \end{pmatrix} \right\|_{\mathbb{C} \oplus L^2(S^1)}^2. \quad (6.5)$$

Similar to [12, Lemma A.3], the space $\mathcal{V}^{\text{ext}} := \mathcal{X}^2 \otimes \mathcal{Y}^1 \cap \mathcal{X}^1 \otimes \mathcal{Y}^2$ with

$$\mathcal{X}^2 := \mathbb{C} \oplus H^+(S^1), \quad \left\langle \begin{pmatrix} f_0 \\ F \end{pmatrix}, \begin{pmatrix} g_0 \\ G \end{pmatrix} \right\rangle_{\mathcal{X}^2} := f_0 \overline{g_0} + \langle F, G \rangle_{L^2(S^1)}, \quad (6.6a)$$

$$\begin{aligned} \mathcal{X}^1 &:= \text{completion of } \mathbb{C} \oplus H^+(S^1) \text{ w.r.t.} \\ &\quad \left\langle \begin{pmatrix} f_0 \\ F \end{pmatrix}, \begin{pmatrix} g_0 \\ G \end{pmatrix} \right\rangle_{\mathcal{X}^1} := \left\langle \mathcal{T}_- \begin{pmatrix} f_0 \\ F \end{pmatrix}, \mathcal{T}_- \begin{pmatrix} g_0 \\ G \end{pmatrix} \right\rangle_{L^2(S^1)}, \end{aligned} \quad (6.6b)$$

$$\mathcal{Y}^1 := L^2(\tilde{\Gamma}), \quad \mathcal{Y}^2 := H^1(\tilde{\Gamma}) \quad (6.6c)$$

and

$$\left\langle \begin{pmatrix} f_0 \\ F \end{pmatrix}, \begin{pmatrix} g_0 \\ G \end{pmatrix} \right\rangle_{\mathcal{V}^{\text{ext}}} := \left\langle \begin{pmatrix} f_0 \\ F \end{pmatrix}, \begin{pmatrix} g_0 \\ G \end{pmatrix} \right\rangle_{\mathcal{X}^2 \otimes \mathcal{Y}^1} + \left\langle \begin{pmatrix} f_0 \\ F \end{pmatrix}, \begin{pmatrix} g_0 \\ G \end{pmatrix} \right\rangle_{\mathcal{X}^1 \otimes \mathcal{Y}^2} \quad (6.6d)$$

is a Hilbert space and fulfills the requirements of the Hardy space method. Note, that

$$\mathcal{V}^{\text{ext}} \subset (\mathbb{C} \oplus H^+(S^1)) \otimes L^2(\tilde{\Gamma}) \sim L^2(\tilde{\Gamma}) \oplus (H^+(S^1) \otimes L^2(\tilde{\Gamma})).$$

We will denote elements of \mathcal{V}^{ext} in the second form, i.e. $\begin{pmatrix} v_0 \\ V \end{pmatrix} \in \mathcal{V}^{\text{ext}}$ with $v_0 \in L^2(\tilde{\Gamma})$ and $V \in H^+(S^1) \otimes L^2(\tilde{\Gamma})$. Recall from [12, Lemma A.1] the identity

$$\int_0^\infty f(x) g(x) dx = \frac{-i\kappa_0}{\pi} \int_{S^1} (\mathcal{M}_{\kappa_0} \mathcal{L} f)(z) (\mathcal{M}_{\kappa_0} \mathcal{L} g)(\bar{z}) |dz|, \quad (6.7)$$

which is applicable for $u(\bullet, y)$, $v(\bullet, y)$ as well as $\partial_x u(\bullet, y)$ and $\partial_x v(\bullet, y)$ and all $y \in \tilde{\Gamma}$. Using the involution $\mathcal{C} : H^+(S^1) \rightarrow H^+(S^1)$ defined by $(\mathcal{C} F)(z) := F(\bar{z})$ for $z \in S^1$ and $F \in H^+(S^1)$ as in [12] we get

$$\int_{S^1} (\mathcal{M}_{\kappa_0} \mathcal{L} f)(z) (\mathcal{C} \mathcal{M}_{\kappa_0} \mathcal{L} g)(\bar{z}) |dz| = \langle \mathcal{M}_{\kappa_0} \mathcal{L} f, \mathcal{M}_{\kappa_0} \mathcal{L} g \rangle_{L^2(S^1)}.$$

Hence, the exterior Hardy space sesquilinear forms for one waveguide are

$$\begin{aligned} a^{\text{ext}} \left(\begin{pmatrix} u_0 \\ U \end{pmatrix}, \begin{pmatrix} v_0 \\ V \end{pmatrix} \right) &:= \frac{-i\kappa_0}{\pi} \langle (\mathcal{T}_+ \otimes \mathbf{I}_{\tilde{\Gamma}})(u_0, U), (\mathcal{T}_+ \otimes \mathbf{I}_{\tilde{\Gamma}})(v_0, V) \rangle_{L^2(S^1) \otimes L^2(\tilde{\Gamma})} \\ &\quad + \frac{-i\kappa_0}{\pi} \frac{1}{(i\kappa_0)^2} \langle (\mathcal{T}_- \otimes \nabla_{\tilde{\Gamma}})(u_0, U), (\mathcal{T}_- \otimes \nabla_{\tilde{\Gamma}})(v_0, V) \rangle_{H^1(S^1) \otimes L^2_{\tan}(\tilde{\Gamma})}, \\ b^{\text{ext}} \left(\begin{pmatrix} u_0 \\ U \end{pmatrix}, \begin{pmatrix} v_0 \\ V \end{pmatrix} \right) &:= \frac{-i\kappa_0}{\pi} \frac{1}{(i\kappa_0)^2} \langle (\mathcal{T}_- \otimes \mathbf{I}_{\tilde{\Gamma}})(u_0, U), (\mathcal{T}_- \otimes \mathbf{I}_{\tilde{\Gamma}})(v_0, V) \rangle_{H^1(S^1) \otimes L^2(\tilde{\Gamma})}. \end{aligned} \quad (6.8)$$

$L_{\tan}^2(\tilde{\Gamma})$ denotes the space of square integrable tangential vector fields on $\tilde{\Gamma}$. For a single waveguide, the Hardy space variational formulation is to find the solution $(u_0, U) \in \mathcal{V}^{\text{ext}}$ of

$$a^{\text{ext}}\left(\begin{pmatrix} u_0 \\ U \end{pmatrix}, \begin{pmatrix} v_0 \\ V \end{pmatrix}\right) - \kappa^2 b^{\text{ext}}\left(\begin{pmatrix} u_0 \\ U \end{pmatrix}, \begin{pmatrix} v_0 \\ V \end{pmatrix}\right) = F\left(\begin{pmatrix} v_0 \\ V \end{pmatrix}\right), \quad \begin{pmatrix} v_0 \\ V \end{pmatrix} \in \mathcal{V}^{\text{ext}}, \quad (6.9)$$

for one $F \in \mathcal{V}^{\text{ext}*}$.

6.3 convergence of the Hardy space method

Similar to Sec. 5.3 we check the assumptions point by point. For simplicity, we again use Dirichlet boundary condition and only one single waveguide.

Assumption A: Exterior and interior spaces and *Assumption B: separation of \mathcal{V}^{ext}* . Most of these assumptions hold true as in the PML case since we use the same interior space, the same spaces \mathcal{Y}_1 and \mathcal{Y}_2 and the same orthogonal system $\{\varphi_n : n \in \mathbb{N}\} \subset \mathcal{Y}_2$ as in the PML case. The assumptions on \mathcal{V}^{ext} hold true by construction. The boundedness and surjectivity of the trace operator $\text{tr}_+ : \mathcal{V}^{\text{ext}} \rightarrow \mathcal{Z} := H^{1/2}(\tilde{\Gamma})$ defined by

$$\text{tr}_+\left(\begin{pmatrix} v_0 \\ V \end{pmatrix}\right) := v_0, \quad \begin{pmatrix} v_0 \\ V \end{pmatrix} \in \mathcal{V}^{\text{ext}},$$

can be proven similar to [12, Lemma A.3]. The modal exterior sesquilinear forms defined in (3.6) are

$$\begin{aligned} s_n\left(\begin{pmatrix} u_0 \\ U \end{pmatrix}, \begin{pmatrix} v_0 \\ V \end{pmatrix}\right) &:= \frac{-i\kappa_0}{\pi} \langle \mathcal{T}_+\left(\begin{pmatrix} u_0 \\ U \end{pmatrix}\right), \mathcal{T}_+\left(\begin{pmatrix} v_0 \\ V \end{pmatrix}\right) \rangle_{L^2(S^1)} \\ &\quad + (\lambda_n - \kappa^2) \frac{i}{\kappa_0 \pi} \langle \mathcal{T}_-\left(\begin{pmatrix} u_0 \\ U \end{pmatrix}\right), \mathcal{T}_-\left(\begin{pmatrix} v_0 \\ V \end{pmatrix}\right) \rangle_{L^2(S^1)} \end{aligned} \quad (6.10)$$

and the modal spaces are $\mathcal{X}_n := \mathbb{C} \oplus H^+(S^1)$ with

$$\left\langle \begin{pmatrix} u_0 \\ U \end{pmatrix}, \begin{pmatrix} v_0 \\ V \end{pmatrix} \right\rangle_{\mathcal{X}_n} := u_0 \overline{v_0} + \langle U, V \rangle_{L^2(S^1)} + (1 + \lambda_n) \langle \mathcal{T}_-\left(\begin{pmatrix} u_0 \\ U \end{pmatrix}\right), \mathcal{T}_-\left(\begin{pmatrix} v_0 \\ V \end{pmatrix}\right) \rangle_{L^2(S^1)}. \quad (6.11)$$

Assumption C: boundedness and coercivity. Continuity of s_n independent of n follows with the continuity of \mathcal{T}_{\pm} . For the coercivity, we have due to (6.5) the same situation as in the PML case with $\sigma := i/\kappa_0$. Hence, M and $\theta_1, \dots, \theta_n$ are exactly the same as for the PML case and the coercivity constant α differs only by a positive constant (independent of n) from the constant in the PML case.

Assumption D: discrete subspaces. We choose the interior finite element space $\mathcal{V}_h^{\text{int}}$ as in section 2 and $\mathcal{Y}_h := \text{tr}_- \mathcal{V}_h^{\text{int}}$. Since the trigonometric monomials are an orthogonal basis of $H^+(S^1)$, we choose $\mathcal{X}_N := \mathbb{C} \oplus \text{span}\{z^0, \dots, z^{N-2}\} \subset \mathbb{C} \oplus H^+(S^1)$.

Assumption E: eigenproblem setting. The argument is again very similar to that for PML.

Since all assumptions to Theorem 3.2 are fulfilled, we have the following convergence theorem.

Theorem 6.3 (HSM for diffraction problems). *Let $\kappa_0^l \in \mathbb{C}$ with $\Re(\kappa_0^l), \Im(\kappa_0^l) > 0$ for $l = 1, \dots, L$ and $\kappa \in \mathbb{C}$ with $\Re(\kappa) > 0$, $\Im(\kappa) \leq 0$, $\kappa^2 \notin \bigcup_{l=1}^L \sigma(-\Delta_l)$ and $\Lambda := \bigcap_{l=1}^L \Lambda_{\Delta_l}^{i/\kappa_0^l}$. If $\kappa \in \Lambda$ is not a resonance, then equation (5.10) with the exterior Hardy space sesquilinear forms of (6.8) is uniquely solvable with solution $(u^{\text{int}}, u^{\text{ext}})^\top \in \mathcal{V}$, and there exists a constant $h_0 > 0$ such that the discrete variational problems*

$$a\left(\begin{pmatrix} u_h^{\text{int}} \\ u_{h,N}^{\text{ext}} \end{pmatrix}, \begin{pmatrix} v_h^{\text{int}} \\ v_{h,N}^{\text{ext}} \end{pmatrix}\right) - \kappa^2 b\left(\begin{pmatrix} u_h^{\text{int}} \\ u_{h,N}^{\text{ext}} \end{pmatrix}, \begin{pmatrix} v_h^{\text{int}} \\ v_{h,N}^{\text{ext}} \end{pmatrix}\right) = F\left(\begin{pmatrix} v_h^{\text{int}} \\ v_{h,N}^{\text{ext}} \end{pmatrix}\right), \quad \begin{pmatrix} v_h^{\text{int}} \\ v_{h,N}^{\text{ext}} \end{pmatrix} \in \mathcal{V}_{h,N} \quad (6.12)$$

have a unique solution $(u_h^{\text{int}}, u_{h,N}^{\text{ext}})^\top \in \mathcal{V}_{h,N}$ for all $h \leq h_0$ and all $N \in \mathbb{N}$. Moreover, there exists a constant $C > 0$ independent of h and N such that

$$\left\| \begin{pmatrix} u^{\text{int}} \\ u^{\text{ext}} \end{pmatrix} - \begin{pmatrix} u_h^{\text{int}} \\ u_{h,N}^{\text{ext}} \end{pmatrix} \right\|_{\mathcal{V}} \leq C \inf_{(w_h^{\text{int}}, w_{h,N}^{\text{ext}})^\top \in \mathcal{V}_{h,N}} \left\| \begin{pmatrix} u^{\text{int}} \\ u^{\text{ext}} \end{pmatrix} - \begin{pmatrix} w_h^{\text{int}} \\ w_{h,N}^{\text{ext}} \end{pmatrix} \right\|_{\mathcal{V}}.$$

Theorem 6.4 (HSM for resonance problems). *Let Λ be defined as in Theorem 6.3. Then for all compact $\Lambda' \subset \Lambda$ we have*

$$\lim_{h \rightarrow 0, N \rightarrow \infty} \text{dist}(\Sigma \cap \Lambda', \Sigma_{h,N} \cap \Lambda') = 0.$$

There is no truncation error in the Hardy space method. Nevertheless, if $\kappa^2 \approx \lambda_n$ for some n the approximation error can be large: For a single waveguide U is given by (see (6.1) together with (6.4))

$$U(z, y) = \sum_{n=1}^{\infty} \frac{\tilde{c}_n}{1/\zeta_n - z} \varphi_n(y) = \sum_{n=1}^{\infty} \tilde{c}_n \varphi_n(y) \sum_{j=0}^{\infty} \zeta_n^{j+1} z^j \text{ with } \zeta_n := \frac{\kappa_n - \kappa_0}{\kappa_n + \kappa_0}. \quad (6.13)$$

W.l.o.g. we assume $(\tilde{c}_n)_n$ to be exponentially decaying. This is always the case, if there exists a positive distance a of Γ to a source of the scattered wave due to the exponentially decaying evanescent modes $e^{i\kappa_n a}$. With (6.2) we have $|\zeta_n| < 1$ and we can estimate the square of the exterior approximation error for each mode $(u_{0,n}, U_n)^\top \in \mathcal{X}_n$ by

$$\begin{aligned} & (1 + \lambda_n) \inf_{v_0 \in \mathbb{C}} |u_{0,n} - v_0|^2 + (3 + 2\lambda_n) \inf_{V \in \{z^0, z^1, \dots, z^N\}} \|U_n - V\|_{L^2(S^1)}^2 \\ &= (3 + 2\lambda_n) |\tilde{c}_n|^2 \sum_{j=N+1}^{\infty} |\zeta_n|^{2(j+1)} = \frac{(3 + 2\lambda_n) |\tilde{c}_n|^2 |\zeta_n|^{2(N+2)}}{1 - |\zeta_n|^2}. \end{aligned} \quad (6.14)$$

For fixed n we see an exponential decay with increasing number of degrees of freedom $N+2$. For fixed N , exponential convergence in n follows with exponentially decreasing $(\tilde{c}_n)_n$ and $\lambda_n \in \mathcal{O}(n^2)$, since for $n \rightarrow \infty$

$$\frac{(3 + 2\lambda_n) |\zeta_n|^{2(N+2)}}{1 - |\zeta_n|^2} \leq \tilde{C} \frac{3 + 2\lambda_n}{|1 - \zeta_n|^2} = \frac{\tilde{C}}{4|\kappa_0|^2} (3 + 2\lambda_n) |\sqrt{\kappa^2 - \lambda_n} + \kappa_0|^2.$$

Similar to the PML error, the error becomes large, if $|\zeta_n| \approx 1$ for one $n \in \mathbb{N}$, which is the case for $\kappa^2 \approx \lambda_n$ (i.e. $\zeta_n \approx -1$) and near the branch cuts of the square root for κ_n .

6.4 Modified Hardy space method

Nevertheless, for diffraction problems with given frequency and given wavenumbers we are able to modify the HSM slightly to get rid of the problem for $\kappa^2 \approx \lambda_n$, i.e. $|\kappa_n|$ small and $|\zeta_n| \approx 1$ in (6.13). The problem arises since the approximation of the mode

$$b_\zeta(z) := \frac{1}{1 - \zeta z} = \sum_{j=0}^{\infty} \zeta^j z^j$$

with the monomials z^0, \dots, z^N is bad for $|\zeta| \approx 1$. Hence, if κ_n and therefore ζ_n is known and if one of the $|\zeta_n|$ is near to 1, it seems reasonable to include this critical mode to the basis

$$\tilde{\mathcal{X}}_N := \mathbb{C} \oplus \text{span}\{z^0, z^1, \dots, z^N, \frac{1}{1 - \zeta z}\} \subset \mathbb{C} \oplus H^+(S^1).$$

Note that $\zeta_n \rightarrow 1$ for $n \rightarrow \infty$, but since $(\tilde{c}_n)_n$ decreases exponentially, $|\zeta_n| \approx 1$ is only a problem, if this happens for small n .

The discrete operators $\tilde{\mathcal{T}}_{\pm}^N : \tilde{\mathcal{X}}_N \rightarrow \text{span}\{z^0, z^1, \dots, z^N, \frac{1}{1 - \zeta z}\}$ and the usual operators $\mathcal{T}_{\pm}^N : \mathcal{X}_N \rightarrow \text{span}\{z^0, z^1, \dots, z^N, z^{N+1}\}$ are described by the matrices

$$\tilde{\mathcal{T}}_{\pm}^N := \begin{pmatrix} 1 & \pm 1 & 0 & 0 & -\frac{1}{d} \\ 0 & \ddots & \ddots & 0 & 0 \\ 0 & 0 & 1 & \pm 1 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{d} \pm 1 \end{pmatrix}, \quad \mathcal{T}_{\pm}^N := \begin{pmatrix} 1 & \pm 1 & 0 & 0 \\ 0 & \ddots & \ddots & 0 \\ 0 & 0 & 1 & \pm 1 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

We define the bilinear form in (6.7) by

$$q_{\kappa_0}(U, V) := \frac{-i\kappa_0}{\pi} \int_{S^1} U(z) V(\bar{z}) |dz|, \quad U, V \in H^+(S^1).$$

The monomials are orthogonal to each other, and therefore $q_{\kappa_0}(z^j, z^k) = -2i\kappa_0 \delta_{j,k}$. For b_ζ we compute

$$q_{\kappa_0}(b_\zeta, z^j) = -2i\kappa_0 \zeta^j, \quad q_{\kappa_0}(b_\zeta, b_\zeta) = \frac{-2i\kappa_0}{1 - \zeta^2}.$$

If we define the matrices M_{κ_0} , \tilde{M}_{κ_0} , S_{κ_0} and \tilde{S}_{κ_0} by

$$(M_{\kappa_0})_{jk} := \frac{1}{(i\kappa_0)^2} q_{\kappa_0}(\mathcal{T}_{-}^N b_j, \mathcal{T}_{-}^N b_k), \quad (S_{\kappa_0})_{jk} := q_{\kappa_0}(\mathcal{T}_{+}^N b_j, \mathcal{T}_{+}^N b_k)$$

for $b_j, b_k \in \mathcal{X}_N$ and $b_j, b_k \in \tilde{\mathcal{X}}_N$ respectively, we get for the usual Hardy space method

$$M_{\kappa_0} := \frac{2i}{\kappa_0} (\mathcal{T}_{-}^N)^T \mathcal{T}_{-}^N, \quad S_{\kappa_0} := -2i\kappa_0 (\mathcal{T}_{+}^N)^T \mathcal{T}_{+}^N$$

and for the modified one

$$\tilde{M}_{\kappa_0} := \frac{2i}{\kappa_0} (\tilde{\mathcal{T}}_{-}^N)^T D \tilde{\mathcal{T}}_{-}^N, \quad \tilde{S}_{\kappa_0} := -2i\kappa_0 (\tilde{\mathcal{T}}_{+}^N)^T D \tilde{\mathcal{T}}_{+}^N$$

with

$$D := \begin{pmatrix} 1 & 0 & \cdots & 0 & \zeta^0 \\ 0 & \ddots & & & \zeta^1 \\ \vdots & & \ddots & & \vdots \\ 0 & & & 1 & \zeta^N \\ \zeta^0 & \zeta^1 & \cdots & \zeta^N & \frac{1}{1-\zeta^2} \end{pmatrix}.$$

This modification of the Hardy space method is covered by our theory if $|\zeta| \neq 1$. It improves the approximation error a lot, if $|\zeta| \approx 1$. The condition of the system matrix will become large if $|\zeta|$ is not in the neighborhood of 1 since then the extra basis function is well approximated by the other basis functions.

Remark 6.5. *There exist strategies to improve the PML in the case of small effective damping as well. In [29] an adaptive procedure to chose the thickness of the damping layer is presented, which was amongst others used for the simulation of a 3d plasmonic waveguide [4]. Moreover, at least for positive κ the mesh in the damping layer should be coarser with increasing x , since typically the highly oscillating waves ($\Re(\kappa_n)$ large) needing a fine mesh are damped out quickly.*

7 Numerical Results

There exist several numerical studies for diffraction and resonance problems for two-dimensional waveguide problems using PML and Hardy space methods [9, 10]. Here, we confine ourselves to one detailed convergence study for a 3d diffraction problem and one numerical computation of a resonance problem. All the computations were done in the finite element code Netgen/NGsolve [27] using openMP parallelization with the direct solver PARDISO [26] or MPI parallelization with the sparse direct solver MUMPS.

7.1 Scattering problem

We consider a single tube $\Omega := \mathbb{R} \times \tilde{\Gamma}$ with the unit disk $\tilde{\Gamma} := B_1(0) \subset \mathbb{R}^2$ as cross section and homogeneous Neumann boundary conditions $\mathcal{B}u = \frac{\partial u}{\partial \nu} = 0$ on $\partial\Omega$. The interior domain was chosen as $\Omega_{\text{int}} := (0, 1) \times B_1(0)$, and the two components of the exterior domain $\Omega_{\text{ext}} = W_1 \cup W_2$ are $W_1 := (1, \infty) \times B_1(0)$ and $W_2 := (-\infty, 0) \times B_1(0)$. The eigenfunctions of $-\Delta : \{\varphi \in H^2(\tilde{\Gamma}) : \frac{\partial \varphi}{\partial \nu} = 0 \text{ on } \partial\tilde{\Gamma}\} \rightarrow L^2(\tilde{\Gamma})$ are

$$\varphi_{\pm m, n}(r \cos \theta, r \sin \theta) = J_m(\mu_{m, n} r) e^{\pm i m \theta}, \quad m \in \mathbb{N}_0, n \in \mathbb{N}.$$

J_m are the Bessel functions and $\mu_{m, n}$ the n th root of J'_m . The first corresponding eigenvalues are $\lambda_1 = \mu_{0, 1}^2 = 0$,

$$\begin{aligned} \lambda_2 = \lambda_3 = \mu_{1, 1}^2 &\approx 1.84118378134^2, & \lambda_4 = \lambda_5 = \mu_{2, 1}^2 &\approx 3.05423692823^2, \\ \lambda_6 := \mu_{0, 2}^2 &\approx 3.83170597021^2, & \lambda_7 = \lambda_8 := \mu_{3, 1}^2 &\approx 4.20118894121^2. \end{aligned}$$

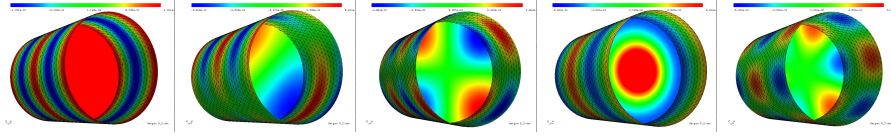


Figure 3: 5 waveguide modes to the surface eigenvalues $\lambda_1, \lambda_2, \lambda_4, \lambda_6$ and λ_7 for $\kappa = 5$ and $\tilde{\Gamma} = B_1(0)$

For all the computations we have chosen as incoming wave a superposition of 5 waveguide modes (see Fig. 3 for the real part of the modes) using the eigenfunctions to the first 5 eigenvalues neglecting the multiplicities:

$$u_{\text{inc}}(x, y) := \sum_{n \in \{1, 2, 4, 6, 7\}} e^{i\sqrt{\kappa^2 - \lambda_n}x} \varphi_n(y), \quad x \in \mathbb{R}, y \in \tilde{\Gamma}.$$

The interior domain for all computations in this subsections is $\Omega_{\text{int}} = (0, 1) \times B_1(0)$ and discretized by 17750 tetrahedrons with maximal mesh size $h = 0.1$.

First, we analyze the dependence of the error of the Hardy space method on the complex parameter κ_0 . Neglecting the compact perturbation arguments in the proof of Theorem 3.2 the theoretical error bound of (6.14) is

$$\eta(\kappa_0, \kappa, N) := \frac{C(\kappa_0, \kappa)}{\alpha(\kappa_0, \kappa)} \sqrt{\sum_{n \in \{1, 2, 4, 6, 7\}} \frac{(3 + 2\lambda_n) |e^{i\kappa_n(\kappa)}|^2 |d_n(\kappa_0, \kappa)|^{2(N+2)}}{1 - |d_n(\kappa_0, \kappa)|}}, \quad (7.1)$$

with $\alpha(\kappa_0, \kappa) := \min\{\alpha_1(\kappa_0, \kappa), \dots, \alpha_5(\kappa_0, \kappa)\}$ and

$$\begin{aligned} C(\kappa_0, \kappa) &:= \frac{4}{\pi} \max \left\{ |\kappa_0| + \left| \frac{\kappa^2}{\kappa_0} \right|, \frac{1}{|\kappa_0|} \right\}, \\ \alpha_n(\kappa_0, \kappa) &:= \frac{1}{\pi} \begin{cases} \min \left\{ \Re(\kappa_0), \Re\left(\frac{\lambda_n^2 - \kappa^2}{\kappa_0(1 + \lambda_n)}\right) \right\}, & \Re\left(\frac{\lambda_n^2 - \kappa^2}{\kappa_0(1 + \lambda_n)}\right) > 0, \\ \min \left\{ \Im(\kappa_0), \Im\left(\frac{\lambda_n^2 - \kappa^2}{\kappa_0(1 + \lambda_n)}\right) \right\}, & \Re\left(\frac{\lambda_n^2 - \kappa^2}{\kappa_0(1 + \lambda_n)}\right) \leq 0 \end{cases}, \\ d_n(\kappa_0, \kappa) &:= \frac{\kappa_n(\kappa) - \kappa_0}{\kappa_n(\kappa) + \kappa_0}. \end{aligned}$$

We tested three different frequencies with a sufficiently fine finite element discretization such that the error of the Hardy space method was dominating. The results shown in Fig. 4 demonstrate that the bound (7.1) represents the dependence of the error on the parameter κ_0 qualitatively correctly and would provide a good guidance for the choice of κ_0 in this example.

Let us discuss that last two frequencies in Fig. 4 which are very special. $\kappa = 4.2$ is in the neighborhood of $\sqrt{\lambda_7}$, and hence the error of the standard HSM is large even with 20 degrees of freedom in radial direction (cf. Fig. 5(b)). Moreover, it can clearly be seen in this case that the optimal parameter κ_0 depends on the wavenumbers κ_n . The

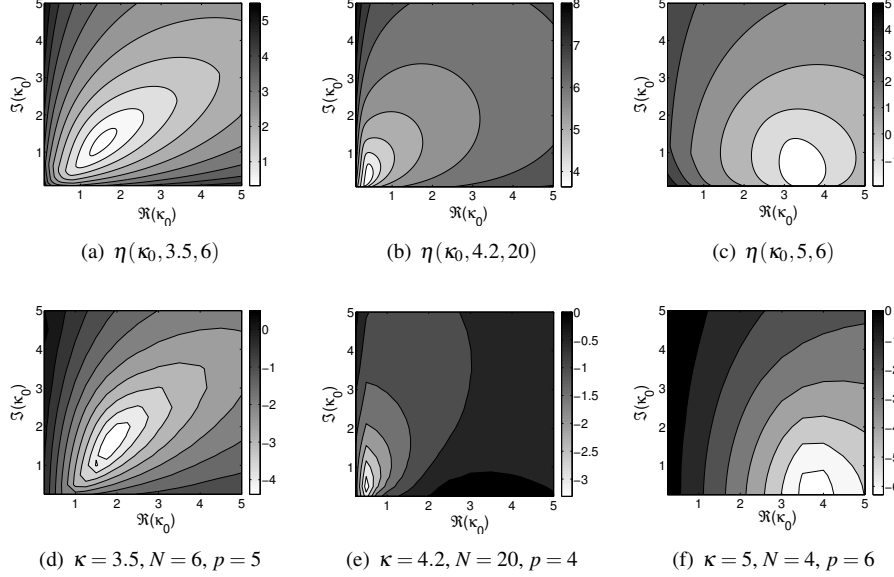


Figure 4: Study of the dependence of the error of the HSM on the complex parameter κ_0 . The upper panels show $\log_{10} \eta$ where η is approximate error bound in (7.1). The lower panel shows $\log_{10} \|u_h^{\text{int}} - u^{\text{int}}\|_{H^1(\Omega_{\text{int}})}$.

”problematic” wavenumber $\kappa_5 \approx 0.1i$ is very small and therefore the optimal parameter κ_0 of the standard HSM would be very small. The modified HSM of Sec. 6.4 resolves this problem completely (see Fig. 5(b)).

The test for $\kappa = 5$ in Fig. 4 is also special, since for $\kappa > \sqrt{\lambda_7}$ all 5 used modes are guided and no evanescent mode has to be resolved by the Hardy space method. Hence, the optimal κ_0 would be almost real and only very few degrees of freedoms in radial direction are necessary ($N = 4$ for a polynomial order $p = 6$). This case would happen in a practical computation if the distance of the artificial boundary $\{1\} \times \tilde{\Gamma}$ to a source or a scatterer is large since then the evanescent modes are already damped out at $\{1\} \times \tilde{\Gamma}$.

Second, we have fixed the parameter $\kappa_0 = 2 + 2i$ and computed the relative $H^1(\Omega_{\text{int}})$ -error for different finite element polynomial orders and different numbers N of degrees of freedom for the Hardy space method (see Fig. 5(a)). In the left panel the exponential convergence of the Hardy space method can be seen. For the most expensive computation with $N = 14$ and $p = 6$, we have used the MPI parallel sparse direct solver MUMPS with 30 cores and in total 1 million unknowns. Approx. 30% of these unknowns were needed for the Hardy space method. The wall time for this computation was approximately 39 minutes, 37 of them spent for the MUMPS factorization.

Last, we have computed dependence of the error on the frequency κ with fixed $\kappa_0 = 2 + 2i$, $N = 10$, and fixed finite element discretization. In Sec. 6.4 we have already

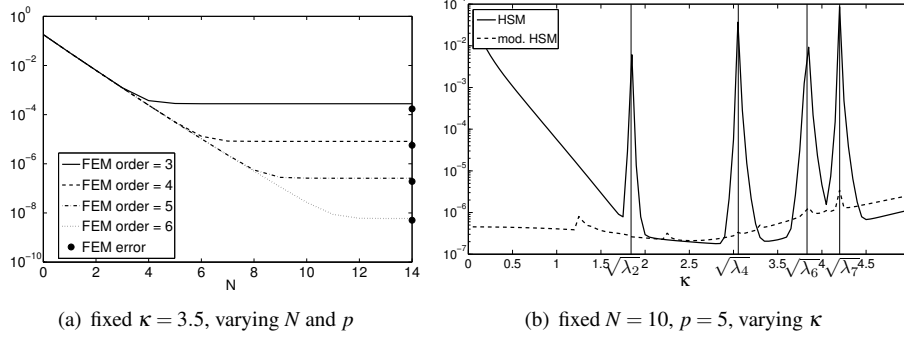


Figure 5: relative $H^1(\Omega_{\text{int}})$ -error for $\kappa_0 = 2 + 2i$. The dots in the left panel represent the pure finite element error with given Dirichlet boundary data. For the modified HSM see Sec. 6.4.

mentioned the problem with $\kappa^2 \approx \lambda_n$, which can be seen in Fig. 5(b). The modified Hardy space method of Sec. 6.4 resolves the problem completely. However, this modification cannot easily be used for resonance problems since it would lead to nonlinear eigenvalue problems.

7.2 Resonance problem

There exist numerical convergence studies to acoustic and electromagnetic resonance problems using the Hardy space method in [21, 22]. Here, we only present one simple 3d resonance problem, which is an extension of the 2d waveguide cavity problems in [10]. The domain is given by a circular ring cavity of radius 2 and length 1 connected with two circular waveguides with radius 1: $\Omega = (-\infty, -0.5) \times B_1(0) \cup (-0.5, 0.5) \times B_2(0) \cup (0.5, \infty) \times B_1(0)$.

We chose $\Omega_{\text{int}} := \Omega \cap (-1, 1) \times B_2(0)$ and discretized the resonance problem with a finite element mesh with maximal mesh size $h = 0.5$ and 654 volume elements, isoparametric elements of order $p = 14$ and the Hardy space method for the two waveguides with $\kappa_0 = 2 + 2i$ and $N = 25$. The first 1000 resonances computed with a shift and invert Arnoldi algorithm with fixed shift $\rho = 10 - i$, the sparse direct solver MUMPS and a Krylov space of dimension 2000 are given in Fig. 6.

For a closed cylinder of length 1 and radius 2 the resonances are

$$\kappa_{m,n,l} = \sqrt{\left(\frac{\mu_{m,n}}{2}\right)^2 + (l\pi)^2}, \quad m, l \in \mathbb{N}_0, n \in \mathbb{N}. \quad (7.2)$$

The resonance functions in Fig. 7 are perturbations of the closed cavity eigenfunctions (compare the resonance function in Fig. 7(a) with the second mode in Fig. 3). For a complex resonance, the imaginary part reflects the energy loss per cycle. Since the only possible energy loss is the energy radiated to infinity and since only guided modes radiate energy to infinity (see Sec. 2), the resonances are real, if the resonance function

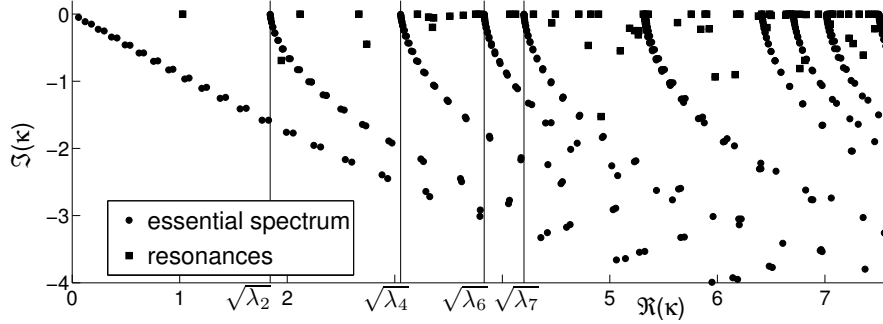


Figure 6: Computed resonances of a circular ring cavity, see Fig. 7. With dots we indicate the discretization of the continuous spectrum (see e.g. [16] for the analogous situation of PML with $\sigma = i/\kappa_0$). They build the boundary of the admissible set (cf. Fig. 6 with Fig. 2). The boxes indicate computed resonances.

is orthogonal to the finitely many guided modes. This is the case in panel (a): For $\Re(\kappa) < \sqrt{\lambda_2}$ only the plane wave is guided and since the resonance function is antisymmetric with respect to the centerline of the waveguide, it is orthogonal to all guided modes. This suggests that the imaginary part of the computed resonance k_1 is a numerical error.

These computations show that resonances in domains including open waveguides can be computed naturally and reliably by the Hardy space method since it leads to a discrete eigenvalue problem. In contrast, methods which rely on a modal decomposition lead to discrete system which depend on the unknown κ in a much more complicated way.

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References

- [1] É. BÉCACHE, A.-S. BONNET-BENDHIA, AND G. LEGENDRE, *Perfectly matched layers for the convected Helmholtz equation*, SIAM Journal on Numerical Analysis, 42 (2004), pp. 409–433.
- [2] J.-P. BERENGER, *A perfectly matched layer for the absorption of electromagnetic waves*, J. Comput. Phys., 114 (1994), pp. 185–200.

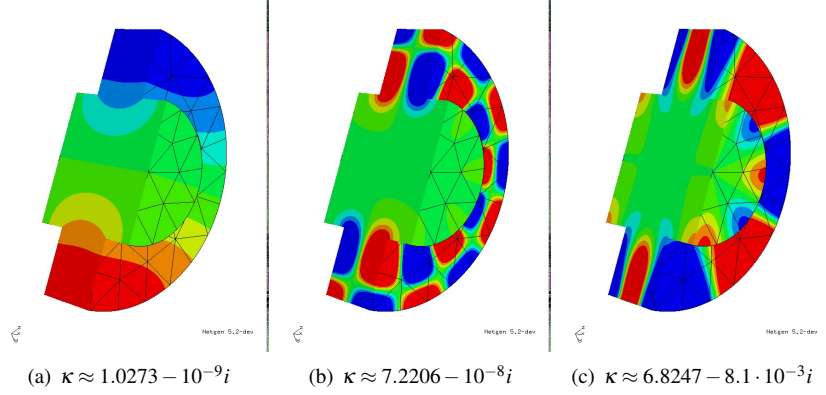


Figure 7: The real part of 3 resonance functions of a circular ring cavity are displayed (cf. Fig. 7). These resonances correspond to the following eigenvalues of the closed cylinder (see (7.2)): (a): $\kappa_{1,1,0} \approx 0.92059$; (b): $\kappa_{7,2,1} \approx 7.18897$; (c): $\kappa_{5,1,2} \approx 6.82257$.

- [3] A. S. BONNET-BEN DHIA, P. CIARLET JR., AND C. M. ZWÖLF, *Time harmonic wave diffraction problems in materials with sign-shifting coefficients*, Journal of Computational and Applied Mathematics, 234 (2010), pp. 1912 – 1919.
- [4] S. BURGER, L. ZSCHIEDRICH, J. POMPLUN, AND F. SCHMIDT, *Finite element method for accurate 3d simulation of plasmonic waveguides*, in Integrated Optics: Devices, Materials, and Technologies XIV, vol. 7604, Proc. SPIE, 2010, p. 76040F.
- [5] Z. CHEN AND H. WU, *An adaptive finite element method with perfectly matched absorbing layers for the wave scattering by periodic structures*, SIAM J. Numer. Anal., 41 (2003), pp. 799–826.
- [6] P. L. DUREN, *Theory of H^p spaces*, Pure and Applied Mathematics, Vol. 38, Academic Press, New York, 1970.
- [7] I. GOHBERG, S. GOLDBERG, AND M. A. KAASHOEK, *Classes of linear operators. Vol. I*, vol. 49 of Operator Theory: Advances and Applications, Birkhäuser Verlag, Basel, 1990.
- [8] W. HACKBUSCH, *Theorie und Numerik elliptischer Differentialgleichungen*, Teubner Studienbücher Mathematik. [Teubner Mathematical Textbooks], B. G. Teubner, Stuttgart, second ed., 1996.
- [9] S. HEIN, W. KOCH, AND L. NANNEN, *Fano resonances in acoustics*, J. Fluid Mech., 664 (2010), pp. 238–264.
- [10] S. HEIN, W. KOCH, AND L. NANNEN, *Trapped modes and Fano resonances in two-dimensional acoustical ductcavity systems*, Journal of Fluid Mechanics, 692 (2012), pp. 257–287.

- [11] P. D. HISLOP AND I. M. SIGAL, *Introduction to spectral theory*, vol. 113 of Applied Mathematical Sciences, Springer-Verlag, New York, 1996. With applications to Schrödinger operators.
- [12] T. HOHAGE AND L. NANNEN, *Hardy space infinite elements for scattering and resonance problems*, SIAM J. Numer. Anal., 47 (2009), pp. 972–996.
- [13] T. HOHAGE, F. SCHMIDT, AND L. ZSCHIEDRICH, *Solving time-harmonic scattering problems based on the pole condition. II. Convergence of the PML method*, SIAM J. Math. Anal., 35 (2003), pp. 547–560.
- [14] V. KALVIN, *Perfectly Matched Layers for diffraction gratings in inhomogeneous media, stability and error estimates*, SIAM J. Appl. Math., 40 (2011), pp. 309–330.
- [15] O. KARMA, *Approximation in eigenvalue problems for holomorphic Fredholm operator functions. I*, Numer. Funct. Anal. Optim., 17 (1996), pp. 365–387.
- [16] S. KIM AND J. E. PASCIAK, *The computation of resonances in open systems using a perfectly matched layer*, Math. Comp., 78 (2009), pp. 1375–1398.
- [17] R. KRESS, *Linear integral equations*, vol. 82 of Applied Mathematical Sciences, Springer-Verlag, New York, second ed., 1999.
- [18] M. LASSAS AND E. SOMERSALO, *On the existence and the convergence of the solution of the pml equations*, Computing, 60 (1998), pp. 229–241.
- [19] M. LEVITIN AND M. MARLETTA, *A simple method of calculating eigenvalues and resonances in domains with infinite regular ends*, Proc. Roy. Soc. Edinburgh Sect. A, 138 (2008), pp. 1043–1065.
- [20] N. MOISEYEV, *Quantum theory of resonances: Calculating energies, width and cross-sections by complex scaling*, Physics reports, 302 (1998), pp. 211–293.
- [21] L. NANNEN, T. HOHAGE, A. SCHÄDLE, AND J. SCHÖBERL, *Exact Sequences of High Order Hardy Space Infinite Elements for Exterior Maxwell Problems*, SIAM J. Sci. Comput., 35 (2013), pp. A1024–A1048.
- [22] L. NANNEN AND A. SCHÄDLE, *Hardy space infinite elements for Helmholtz-type problems with unbounded inhomogeneities*, Wave Motion, 48 (2010), pp. 116–129.
- [23] S. A. NAZAROV AND B. A. PLAMENEVSKY, *Elliptic Problems with Domains with Piecewise Smooth Boundaries*, Walter de Gruyter, Berlin, New York, 1994.
- [24] P. N. RACEC, E. R. RACEC, AND H. NEIDHARDT, *Evanescent channels and scattering in cylindrical nanowire heterostructures*, Phys. Rev. B, 79 (2009), p. 155305.

- [25] S. ROTTER, F. LIBISCH, J. BURGDÖRFER, U. KUHL, AND H.-J. STÖCKMANN, *Tunable Fano resonances in transport through microwave billiards*, Phys. Rev. E, 69 (2004), p. 046208.
- [26] O. SCHENK AND K. GÄRTNER, *Solving unsymmetric sparse systems of linear equations with PARDISO*, in Computational science—ICCS 2002, Part II (Amsterdam), vol. 2330 of Lecture Notes in Comput. Sci., Springer, Berlin, 2002, pp. 355–363.
- [27] J. SCHÖBERL, *Netgen - an advancing front 2d/3d-mesh generator based on abstract rules*, Comput. Visual. Sci, 1 (1997), pp. 41–52.
- [28] O. STEINBACH AND G. UNGER, *Convergence analysis of a Galerkin boundary element method for the Dirichlet Laplacian eigenvalue problem*, SIAM J. Numer. Anal., 50 (2012), pp. 710–728.
- [29] L. ZSCHIEDRICH, R. KLOSE, A. SCHÄDLE, AND F. SCHMIDT, *A new finite element realization of the Perfectly Matched Layer method for Helmholtz scattering problems on polygonal domains in 2d*, J. Comput. Appl. Math., 188 (2006), pp. 12 – 32.